UCRL-52532 Vol. 1

Computer automation of continuous-flow analyzers for trace constituents in water Volume 1. Operator instructions

Richard W. Crawford

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April 4, 1979

Lawrence Livermore Laboratory

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Computer automation of continuous-flow analyzers for trace constituents in water Volume 1. Operator instructions

ABSTRACT

This document has been written as an aid to an operator when running continuous flow analyses using the LLL programs. It refers specifically to the Technicon AutoAnalyzer instrument. The system, hardware and software, is described so that the operator can relate to the sequence of operations. The importance of the arrangement of solutions in the automatic sampler is emphasized. All prompts and responses are discussed in detail, including editing features and the various options available. In addition, the output and line-printer programs are described along with special auxiliary programs to be used in troubleshooting.

INTRODUCTION TO THE SYSTEM

SCOPE

This document describes a system for running automated analyses on the Technicon AutoAnalyzer II instrument and, with minor differences, the AutoAnalyzer I. The system consists of the arrangement of samples with the necessary standards, quality-control solutions, and the required software and hardware to perform the desired chemical analysis on a group of samples. Computer prompts, operator responses for input, and operator interaction are discussed as well as the various computer outputs and reports.

To provide flexibility and versatility, the software is quite complex. The various options and editing features are also considered with some examples.

TERMS AND DEFINITIONS

Analyte—A constituent of the sample for which the concentration is being sought.

Blanks—Solution samples consisting of (usually) distilled water.

Calibration standards—Known concentrations spanning the full range that will be encountered in the unknown samples to be run. Five to ten calibration standards are used in a typical run. It is best to have one that is more concentrated than the most concentrated sample expected, as well as one that is less concentrated than the least concentrated sample expected.

Check standards—Duplicates of the calibration standards, which are run once in each QC pattern to verify that the instrument is maintaining its calibration.

Duplicates—Samples that are identical to selected samples that have been previously run.

Reagent blanks—Chemicals (reagents) added to a sample at the time it is taken in order to preserve constituents. If these reagents have the analyte of interest in them, they will contaminate all the samples by the same amount. The reagent blanks are measured in order to correct for this effect.

Samples—Measured portions of the unknown material for which the analysis is desired.

Unknown—An unmodified sample.

Set standard—A sample of known concentration chosen to be more than 50% of full-scale, used to establish the start of the output data and the time interval between samples.

Spikes—Samples to which a known amount of the particular analyte has been added. Spikes are used to ascertain if any other components of the sample are interfering with the results of the analysis.

Discussion of Sample-Wheel Pattern

The operator informs the computer of the order in which the solutions are to be examined by selecting the sequence of solutions to be placed in the sample wheel. The sequence is stored in computer files by using the appropriate responses to computer prompts.

Figure 1 shows the sample-wheel pattern for two typical wheels. The first wheel is unique and is mounted at the very beginning of a run. *Sample-wheel pattern* refers to the arrangement of the entire group of solutions to be run, including set standards, calibration standards, blanks, check standards, samples, spiked samples, and duplicates. The first sequence (set standards and calibration standards) is called the *calibrate pattern,* which is discussed below. In Fig. 1 the calibrate pattern consists of samples 1–11. (Each position number represents a tube of solution sample.) The second sequence (samples 12–25, 26–39, 41–52, 54–63 in Fig. 1) consists of blanks, check standards, samples, spiked samples, and duplicates, and is called the *quality-control pattern,* or *QC pattern,* which is also discussed below. The exact QC pattern is established when the operator runs TAAIN. A sample-wheel pattern consists of *one* calibrate pattern followed by as many identical QC patterns as are necessary and using as many wheels as are necessary (limited to 300 wheel locations) to run all of the samples in the group.

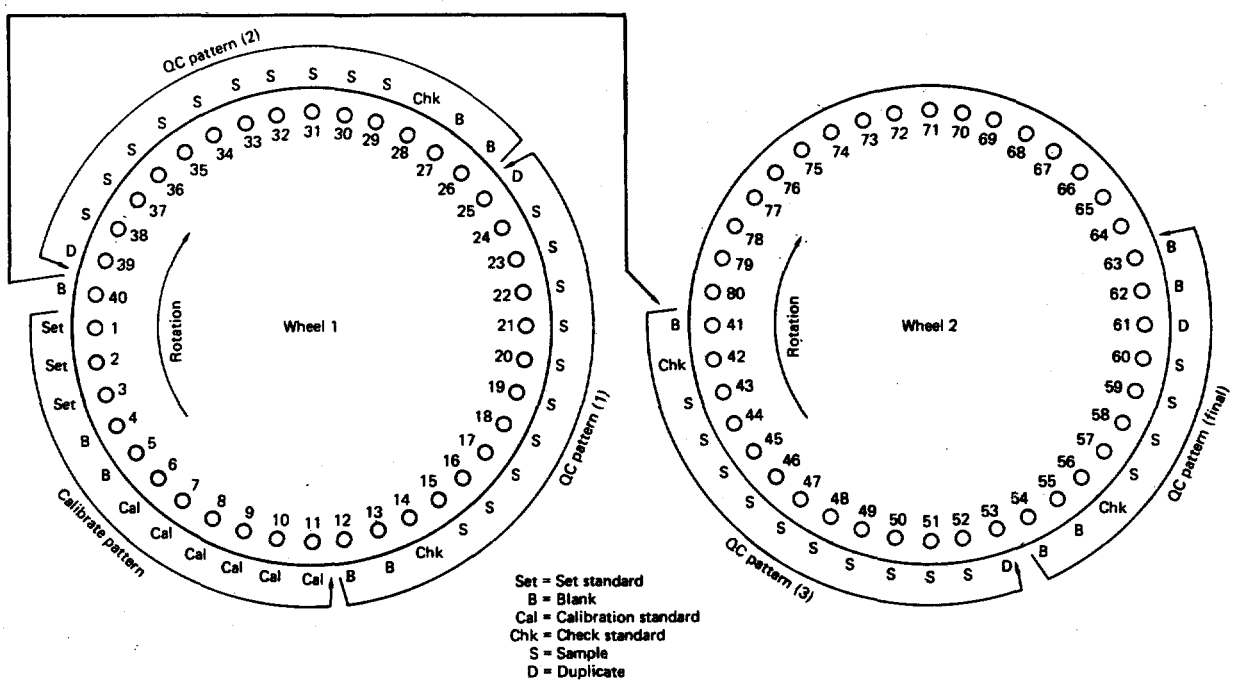


FIG. 1. Typical sample-wheel pattern. Within the calibrate pattern (positions 1–11) are the set standards (positions 1–3), which are used to establish instrument timing, followed by two blanks (positions 4–5), which are used to establish the baseline, followed by six calibration standards (positions 6–11), which are used to relate A/D output to concentration. The first QC pattern (positions 12–25) is made up of two blanks (12–13) used to maintain the baseline, a check standard (14) to verify if the instrument is still in calibration, ten unknown samples (15–24), and one duplicate sample (25) to compare with a previously run unknown. Subsequent QC patterns (26–39, 41–53, 54–63) repeat the order of blanks, check standards, samples, and duplicates, but usually with different samples. Note that the final QC pattern must end with two blanks.

Data may be stored on up to nine standard sample-wheel patterns, all with the same structure. All data, except sample identification numbers (IDs) and dilution factors, are common to all nine sample-wheel patterns. Two files are used to store the data: TAAID for sample IDs and dilution factors, and TAAINF for all other data.

Calibrate Pattern

The beginning sequence of solutions in the sample-wheel pattern is the calibrate pattern. The first three solutions must be set standards, which are used to establish the system timing. They must be at least 5Ø% of full-scale in concentration so that they are not confused with noise. The next two solutions must be blanks, and are used to establish the baseline. These are followed by a series of calibration standards. Figure 1 shows six calibration standards; no specific number of them is required, and no more than 1Ø are allowed. Four or five are recommended.

QC Pattern

The quality-control patterns that follow the calibrate pattern must be identical except for the last one. The first two solutions of the QC pattern should be blanks. These are followed by check standards; at least one should be used, and two are recommended, but more may be used if needed. Sample solutions are next in the sequence. There are two groupings of samples that may be used in the QC pattern. One or both may be used, depending on the procedure being followed. The first group consists of a number of samples (chosen by the operator), including some that have been spiked. The second group consists of an operator-chosen number of samples followed by a selected number of duplicates from that group. If both groupings are used they must be loaded into the wheel in the order given above, namely, samples/spiked samples; samples/duplicate samples. For example, the computer prompt for the QC pattern is*:

QCP	BLK	CS	SAMP	SPK	SAMP	DUP
	? *2*	? *2*	? *1Ø*	? *1*	? *1Ø*	? *2*

The operator has responded (after each question mark) 2 blanks, 2 check standards, 1Ø samples + 1 spike, and 1Ø samples + 2 duplicates. The responses for the QC pattern shown in Fig. 1 would have been as follows:

QCP	BLK	CS	SAMP	SPK	SAMP	DUP
	? *2*	? *1*	? *Ø*	? *1*	? *Ø*	? *1*

In this example the operator has chosen not to use samples separated by spiked samples.

The maximum total number of solutions that can be specified for a single QC pattern is 4Ø. If this number is exceeded, an error message will remind the operator. For example:

QCP	BLK	CS	SAMP	SPK	SAMP	DUP
	? *2*	? *3*	? *Ø*	? *Ø*	? *37*	? *3*

PATTERN TOO LARGE, REDUCE NO. SAMPLES TO 32

The prompt will be repeated so that a correction can be made. Remember that *all sample-wheel patterns (1 to 9) will have the same configuration* (with respect to check standards, spikes, and control standards) *established by the operator* when responding to this prompt.

*For purposes of this report, computer prompts will be indicated in type by **boldface**, and user responses will be indicated by *italics*.

Figure 1 also illustrates two properties of wheel patterns: one is that a QC pattern can be continued from one wheel to the next; the second is that the final QC pattern can have fewer samples in it than the operator-established number of samples in the patterns that precede it. Two blanks must follow the last QC pattern to signal the end of the sample-wheel pattern. The computer programs have been designed to recognize these situations.

The sample-wheel pattern is important because all subsequent operations in the automation procedure, from analysis, calculations, and report writing, depend on its systematic structure.

SOFTWARE

The Technicon AutoAnalyzer (TAA) is operated by software consisting of nine programs written in the extended Dartmouth BASIC language. Figure 2 shows a schematic of how these nine programs work together. In addition, there are three supplementary programs written in BASIC, and a patch to the computer operating system written in assembly language.

The software for the Technicon AutoAnalyzer is designed to combine flexibility, ease of use, high computational power, and large data storage capability. In order to fully utilize this *system,* it is important that the operator understand how the system operates. The programs allow the operator to construct the sample-wheel pattern, assign variables, and supply other pertinent data. These programs also perform all calculations based on signals from the TAA colorimeter, reduce data, and produce output reports. Detailed descriptions of all the program segments, including listings, are given in Volume 4, parts 1 through 13.

- **TAAIN** is the initiating program, the one with which the operator will become most familiar. Its major functions are assigning values to variables and storing them in permanent files, storing sample information in temporary files, and correcting or modifying the stored data.
- **TAAINRE** creates a specifically-formatted output of all the input data recorded by TAAIN, which is called the SAMPLE-WHEEL PATTERN. A line-printer copy of this output shows the content of each position of the sample wheel, and includes useful additional information such as concentrations of standards and spikes. The program also includes editing capabilities.
- **TAASTART** checks the hardware to make sure everything is functional and establishes the zero—and full-scale—output readings of the colorimeter. It then starts the real-time program (assembly language) in the search mode, enabling it to search for the first set standard to establish the timing that correlates a peak to the appropriate wheel-pattern location.
- **TAACAL** calibrates the system by recording colorimeter-response values from a series of calibration standards. These response values are used to calculate the coefficients of polynomial equations, or are stored (in order of concentration) for interpolation. First- (linear), second- (quadratic) or third- (cubic) order polynomials are used to convert measured values to concentrations.
- **TAA** records and determines peak heights, and calculates concentrations for samples, blanks, and quality-control standards. It displays sample information and detects noisy or offscale signals.
- **TAAQCOP** calculates and displays data gathered by TAA for blanks and quality-control standards.
- **TAAO1** is the first of the three output programs. It stores the data in temporary files to expedite rapid printing. It also prints a preliminary report of which reagent blanks were used.
- **TAAO2** displays the reagent-blank values and allows the operator to accept, reject, or enter his/her own values. The correction for the reagent blank is applied by the operator if necessary.
- **TAAO3** prints the final report on the line printer using the files created by TAAO1 and corrected by TAAO2. It prints all the information an operator may need, such as peak height and the standard deviation used to determine the peak height. It also gives information necessary to determine the quality of the data, such as the precision of duplicates and the measurement accuracy of check standards and spikes.

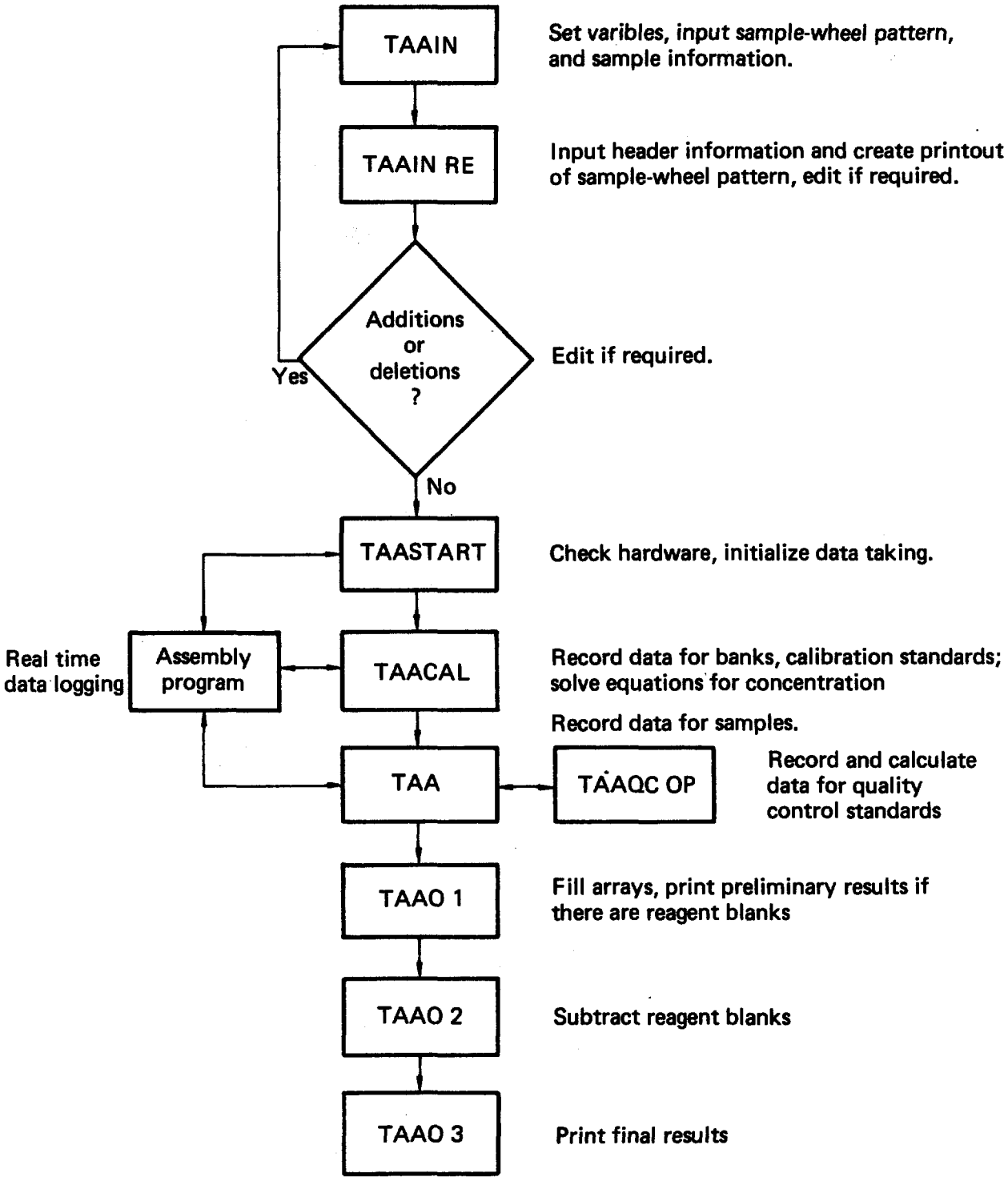


FIG. 2. Overall program flow.

- **Specials** are three short programs available at the end of a run. They are only used occasionally.
  - — **TAAPRINT** is used to print the available results on the line printer if a run is interrupted due to a computer failure or other occurrence that causes an abnormal exit. It sets up necessary variables and then starts up TAAO1 through TAAO3.
  - — **TAAPEAK** allows storage and semi-graphical display of all data taken for each peak. This is especially useful for setting data rates and window widths.
  - — **TAAPFILE** outputs to the line printer the raw data stored in files during a run. It is used only for debugging purposes.
- **Assembly Language (Real-Time) Code** detects and records the actual raw data coming from the colorimeter. It keeps track of the timing of the peaks, and also counts the peaks, and allows corrections in the peak timing to be made using the BASIC programs. See UCRL-52392 for more details.

HARDWARE

Hardware consists of the computer, disks, tape, line printer, terminals, digitizer, and interfaces necessary for the system. Only those pertinent to the TAA operator will be described.

TAA Interface is a box to which the colorimeters are connected, that filters, amplifies, and transmits the signal to the computer, where it is received, attenuated, and filtered. The signal is then directed to an analog-to-digital converter (A/D).

Analog-to-Digital Converter changes the colorimeter analog signal to a digital signal. The A/D is designed for a 10 V full-scale output and has a resolution of 15 bits, or one part in 16,384. Since the output of the TAA is only 5 V, only half this resolution is used. The remaining 5 V is used to provide zero offset (to record negative drift) and to record off-scale samples.

Disks are high-speed, magnetic, digital systems that can reliably store data for six months or more. Although the same disk is used by the TAA program for all data, some files are permanent and others are temporary. The temporary files can be saved if necessary.

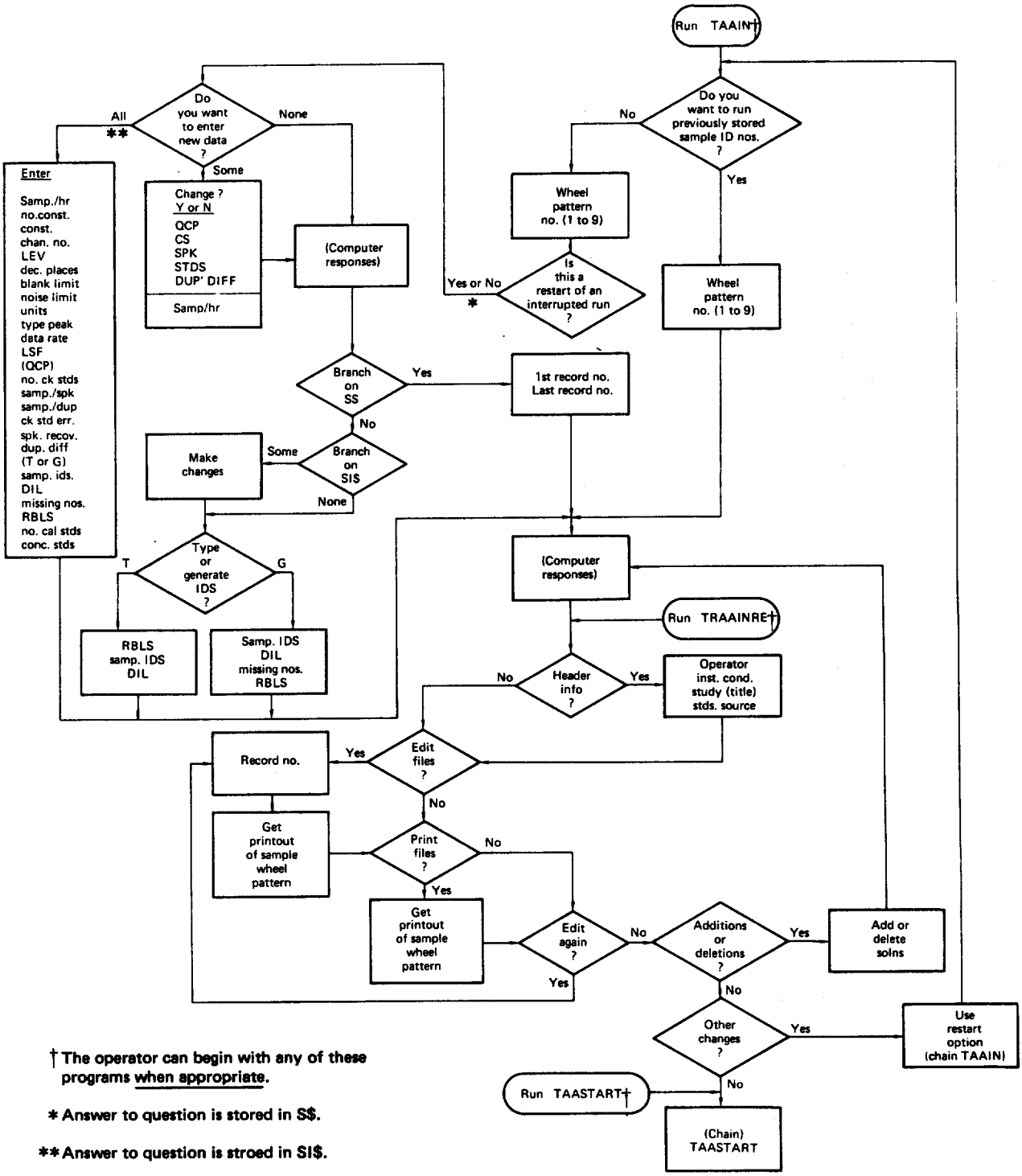
ENTERING DATA USING TAAIN AND TAAINRE

SCOPE

As described in the previous section, the operator must input data to the computer to construct the sample-wheel pattern, assign values to variables, and supply other pertinent information. Although two programs are used to input information, set up files, and get a line-printer copy of the sample-wheel pattern for a run, the operator only interacts with one. TAAIN is the main program for inputs and file construction. It chains to TAAINRE to input the wheel-pattern header information, edit, and print the files. Since inputs and outputs appear to be from the same program, these instructions are written as though they were a single program.

The programs will ask for information in a fixed sequence, wait for operator input, and then generate the wheel pattern. The output results are in a format suitable for the operator to use as a work sheet to load the sample wheels and as a guide during the course of an AutoAnalyzer analysis run. The programs will handle one to six constituents; however, a maximum of only three constituents at a time for a given group of samples can be specified to be run by the existing TAA programs.

Figure 3 provides a schematic of the data-input sequencing that results from the various responses to the computer prompts. The remaining text in this section and this schematic supplement each other.



† The operator can begin with any of these programs when appropriate.

* Answer to question is stored in S$.

** Answer to question is stroed in SI$.

FIG. 3. Flow of data-input prompts and responses.

STARTING UP

Logging On

If the computer is up, terminal on, and the programs on disk file, press the ESC key of the terminal. The computer will respond* with **ACCOUNT-ID.** Type the user ID for the TAAIN program. No characters will appear on the terminal when the ID characters are typed. Press the RETURN key. The ID to be used is defined by your system manager, and depends on the analytes to be determined. The date, time, **SIGN ON,** and the terminal number will appear on the terminal.

Running

The program can now be loaded into the computer from the magnetic disk by either of two commands. For normal use, type *RUN"TAAIN* and press the RETURN key. This will cause the program to be loaded and start running immediately. The program may also be loaded, but will not start, by typing *LOAD"TAAIN* and pressing the RETURN key. The LOAD command is used when one wishes to make program changes, get a listing, or have the program in core without running; the program can then be started by typing *RUN* and depressing the RETURN key.

When the program starts, it will dimension arrays, initialize variables and counters, and start the dialogue. A run for a new group of samples may be set up, an interrupted run restarted, or a continuation of an earlier run may be made where the same constituents are to be determined. Computer prompts are appropriately answered and always followed by a carriage return.

ENTERING DATA FOR A NEW RUN

Discussion

A "new" run is defined as a run for which no previous data have been stored in the computer disk files, as is the case when a new type of analysis is being set up. In well established laboratories, where the same analyses are performed repeatedly using the same sample-wheel pattern, only the sample ID numbers and certain header information need to be changed. Describing a "new" run provides an opportunity to review most of the variables, parameters, and computer prompts encountered when entering data. A complete list of the prompts and responses is shown in Fig. 4.

*As previously noted, computer prompts will appear in **boldface** and user responses will be in *italics.*

ACCOUNT-ID:
Ø3/Ø2/79 Ø8:11 SIGN ON, Ø3
******RUN"TAAIN*
DO YOU WANT TO RUN PREVIOUSLY STORED SAMPLE ID NOS. ? *N*
WHEEL PATTERN NO. (1 TO 9) *1*
IS THIS A RE-START OF AN INTERRUPTED RUN ? *N*
DO YOU WANT TO ENTER NEW DATA
FOR EACH CHAN., QC PATT., STND. CONC., QC LIMITS
ANSWER ALL, SOME, OR NONE (A,S,N) ? *A*
NUMBER OF SAMPLES PER HOUR ? *3Ø*
NO. OF CONSTITUENTS *2*

FIG. 4. Initial operator dialogue—use of G-option.

CONSTITUENTS	CHAN	LEV	PLACES AFTER DEC.	BLK LIM (CONC)	ALLOW NOISE % F S
? *SO4*	? *1*	? *LO*	? *1*	? *2*	? *2*

UNITS OF CONC	TYPE OF PEAK B OR N	DATA RATE 15 TO 60	DEGREE OF LSF 1 TO 4
? *PPM*	? *N*	? *60*	? *2*

INPUT FOR SO4 OK ? *Y*

CONSTITUENT	CHAN	LEV	PLACES AFTER DEC.	BLK LIM (CONC)	ALLOW NOISE % F S
? *CL*	? *2*	? *HI*	? *1*	? *3*	? *2*

UNITS OF CONC	TYPE OF PEAK B OR N	DATA RATE 15 TO 60	DEGREE OF LSF 1 TO 4
? *PPM*	? *B*	? *15*	? *1*

INPUT FOR CL OK? *Y*

QCP	BLK	CS	SAMP	SPK	SAMP	DUP
	? *2*	? *1*	? *5*	? *1*	? *5*	? *1*

PATTERN OK ? *Y*

SO4	CS 1	? *5*	ERR *1*
CL	CS 1	? *20*	ERR *2*

CHECK STDS OK *Y*

SO4	SPK 1	? *5*	MIN *4*	MAX *6*
CL	SPK 1	? *15*	MIN *14*	MAX *16*

SPIKES OK ? *Y*

SO4	DIFF IN DUPS *1*
CL	DIFF IN DUPS *2*

DIFF FOR DUPS OK *Y*

FIG. 4. (cont.)

TYPE OR GENERATE IDS (T OR G) ? *G*

ENTER ID'S AND DIL FOR THE SET

1 ST NO.	LAST NO.	DIL
? *101*	? *120*	? *1*
? *121*	? *130*	? *2*
? *131*	? *140*	? *1*
? *0*		

IDS AND DIL OK ? *Y*

TYPE ALL MISSING SAMPLE NUMBERS

NO. 106
NO. 107
NO. 124
NO. 136
NO. 0

NUMBERS OK ? *Y*

ENTER ALL RBL NOS. AND THE FIRST AND LAST SAMPLE NO. ASSOCIATED

RBL NO.	1 ST SAMP	LAST SAMP
? *105*	? *101*	? *120*
? *125*	? *102*	? *130*
? *135*	? *131*	? *140*
? *0*		

RBLS OK ? *Y*

NO. OF CALIB STDS ? *4*

ENTER CONC OF STDS

SO4	S 1	? *5*	S 2	? *10*	S 3	? *15*	S 4	? *20*
CL	S 1	? *10*	S 2	? *20*	S 3	? *30*	S 4	? *50*

STDS OK ? *Y*

FIG. 4. (cont.)

```
WRITING FILES

  1     PATTERNS COMPLETED
  2     PATTERNS COMPLETED
  3     PATTERNS COMPLETED
 67     FILES IN THIS SET UP
 67     ID FILES IN USE

HEADER INFO ? Y

OPERATOR                        FBS
INSTRUMENT CONDITIONS           OK
STUDY OR GROUP TITLE            TEST 1
STANDARDS SOURCE                FADE DATA-DEMONSTRATION

EDIT FILES ? N
PRINT FILES ? Y
EDIT FILES ? Y
RECORD NO. 44

CONST     TYPE     NO.      DIL      CONC     S1       S2
SO4       RBL      125      2        1        1Ø2      13Ø
                   ? 125    ? 2      ? 1      ? 121    ? 13Ø

CL        RBL
                   125      2        1        1Ø2      13Ø
                   ? 125    ? 2      ? 1      ? 121    ? 13Ø

RECORD NO. Ø
PRINT FILES ? Y
EDIT FILES ? N
ADDITIONS OR DELETIONS ? N
ANY OTHER CHANGES ? N
TAASTART 28Ø9 Ø5/24/77 13:2Ø 8ØØ DC
SET COLORIMETERS TO FULL SCALE, HIT RETURN
SET COLORIMETER TO NORMAL OR PROPER DAMPING, HIT RETURN
STOP AT Ø33Ø
.
```

FIG. 4. (cont.)

Prompts and Responses

The operator logs on by pressing the ESC key and supplying the appropriate ID. Note that the account ID must be typed in but does not appear on printout.

ACCOUNT-ID: _____
Ø3/Ø2/79 Ø8:11 SIGN ON, Ø3

The TAAIN program is then loaded and started by typing:

RUN"TAAIN
DO YOU WANT TO RUN PREVIOUSLY STORED SAMPLE ID NOS. ? *N*

(NOTE: All YES or NO queries can be answered *Y* or *N*. For this example of a new run the logical response is *N*O since no previous data for the run have been stored.)

WHEEL PATTERN NO. (1 TO 9) *1*

Wheel patterns were discussed in the Introduction to the System.

IS THIS A RESTART OF AN INTERRUPTED RUN ? *N*

For this example the response is *N*O. Restarting interrupted runs is discussed on page 48.

DO YOU WANT TO ENTER NEW DATA
FOR EACH CHAN., QC PATT., STND. CONC., QC LIMITS
ANSWER ALL, SOME, OR NONE (A,S,N) ? *A*

A new run will require *A*LL new data to be entered, including sample-wheel-pattern data as well as other (nonsample-wheel-pattern) data. Other data refers to sample rates, error limits, acceptable noise limits, data rate, constituents to be analyzed for, and other necessary "permanent" information.

An examination of Fig. 3 shows the consequences of choosing the SOME or NONE options. The SOME option, generally speaking, allows the operator to enter or change sample-wheel-pattern data for a "normal" run. The NONE option is usually chosen when restarting an interrupted run, or when entering data for a new batch of samples for a "continuing" run (see section on entering data for a continuing run, p. 21).

NUMBER OF SAMPLES PER HOUR ? *3Ø*

The response to this prompt is a function of the automatic sampler rate, which is determined by inserting the appropriate cog wheel into the unit. The value entered is used by a program algorithm to calculate the timing between peaks. The magnitude of the number depends on the complexity of the chemistry, reaction rates, wash-out time, and other physical parameters of the analytical system. [This timing is important. During sample analysis, the computer must anticipate when the next peak is due. Reading data for samples depends primarily on "constant" peak-to-peak timing—not on peak detection (see section on timing change, p. 47). Blanks and very dilute samples may have undetectable peaks, but these data must be taken anyway.]

TABLE 1. Abbreviations used for the different constituents run on Technicon AutoAnalyzers.

Abbreviation	Meaning
NH3	Ammonia
N03N02	Nitrate plus nitrite
NITRITE	Nitrite only
SULFATE	Sulfate from water samples
S02	Bubblers from air program
TKN	Total Kjeldahl nitrogen
CL	Chloride ion
ORTHOP	Orthophosphate
TOTP	Total phosphate
DISP	Dissolved phosphate
COD	Chemical oxygen demand
S102	Silicate ion
ALK	Alkalinity
HG	Mercury
PH	pH, hydrogen ion concentration
PHENOL	Phenols
MBAS	Methylene blue active substances
CN	Cyanide

NO. OF CONSTITUENTS *2*

This prompt requests the number of constituents (analytes) to be determined. In our example, SO_4 and Cl are the constituents, so 2 is the appropriate response.

Immediately after the operator supplies the above response the computer will print a two-line header on the terminal. Below each item of the header a question mark (?) prompts input for each item. The header, with prompts and responses, and a discussion of the responses is given below:

CONSTITUENT	CHAN	LEV	PLACES AFTER DEC.	BLK LIM (CONC)	ALLOW NOISE % F S
? *SO4*	? *1*	? *LO*	? *1*	? *2*	? *2*

- **CONSTITUENT** — input one of the "legal" constituents listed in Table 1. If the analyte is not in the file, a message **ANALYTE NOT IN FILE** will be printed and a new header line will be printed for a new input.
- **CHAN** — enter the A/D channel number for this analyte. An error here cannot be detected, so the operator must be certain that the colorimeter is plugged into the selected channel.
- **LEV** — the expected concentration level or other appropriate data, such as ? *LO* or *HI*. This input is for information only and is not used in any way by the program.
- **PLACES AFTER DEC** — enter the desired significant numbers (up to three) to appear to the right of the decimal in the calculated result for the constituent.
- **BLK LIM (CONC)** — enter the allowable limit for blank drift in units of concentration.
- **ALLOW NOISE % F S** — enter noise allowed for the peak as a percent of full-scale of the recorder. Typical levels are $\emptyset$.2 to 1%.

The computer will again print a two-line header for additional input information, and wait for inputs as before. The items and inputs are:

UNITS OF CONC	TYPE OF PEAK B OR N	DATA RATE 15 TO 60	DEGREE OF LSF 1 TO 4
? *PPM*	? *N*	? *60*	? *2*

- **UNITS OF CONC** — enter the appropriate units, for example, PPM, for parts-per-million.
- **TYPE OF PEAK (B OR N)** — *B*road or *N*arrow, depending on the peak slope and the data rate for this analyte.
- **DATA RATE (15 TO 60)** — enter the data rate in points per minute across the peak top. Thirty-five points are read for each peak.
- **DEGREE OF LSF (1 TO 4)** — enter the type of calculation for this analyte. One stands for linear, 2 quadratic, 3 cubic, and 4 interpolation.

When all the requested data have been entered, the following prompt is given:

INPUT FOR SO4 OK ? *Y*

After checking the data, a *YES* response indicates that correct input has been made for all items. If an error is found on checking the data, a *NO* response will cause the input routine, starting at **CONSTITUENT**, to be repeated and *all* the data must again be entered along with the corrected data.

The above process is repeated for the remaining analytes and is illustrated as follows:

CONSTITUENT	CHAN	LEV	PLACES AFTER DEC.	BLK LIM (CONC)	ALLOW NOISE % F S
? *CL*	? *2*	? *HI*	? *1*	? *3*	? *2*

UNITS OF CONC	TYPE OF PEAK B OR N	DATA RATE 15 TO 60	DEGREE OF LSF 1 TO 4
? *PPM*	? *B*	? *15*	? *1*

INPUT FOR CL OK ? *Y*

If three constituents had been indicated for **NO. OF CONSTITUENTS?** the above procedure would be repeated again for the third analyte.

The next prompt asks for input for the construction of the QC pattern. Its format is the same as those shown previously:

QCP	BLK	CS	SAMP	SPK	SAMP	DUP
	? *2*	? *1*	? *5*	? *1*	? *5*	? *1*

PATTERN OK ? *Y*

- **BLK**—enter the number of blanks desired.
- **CS**—enter the number of check standards desired.
- **SAMP**—enter the number of samples for the first sample group.
- **SPK**—enter the number of samples to be spiked.
- **SAMP**—enter the number of samples in the second sample group.
- **DUP**—enter the number of duplicates to be run in each pattern.

A *NO* response to the confirmation prompt **PATTERN OK?** will require reentering all the QCP data.

A detailed discussion of the quality-control pattern was given in the Introduction. The responses shown here describe the arrangement of the QC pattern for our example. It consists of two blanks, one check standard, five samples plus one duplicate sample. The computer program always chooses the first samples of the associated group for the spikes and duplicates. This is illustrated in the printout of the sample-wheel pattern (Fig. 5).

SO4 **CS 1** ? *5* **ERR** *1*
CL **CS 1** ? *20* **ERR** *2*

CHECK STDS OK? *Y*

Data for the check standards is now entered for each of the analytes. The responses shown above mean that for **SO4**, check standard **#1** has a made-up concentration of *5* ppm and that the value found is allowed an **ERR**or of ±*1* ppm. For **CL**, check standard **#1** has a made-up concentration of *20* ppm and its found value can be in **ERR**or by ±*2* ppm. Additional check standards would require similar input data.

A confirming prompt is also issued.

SO4 **SPK 1** ? *5* **MIN** *4* **MAX** *6*
CL **SPK 1** ? *15* **MIN** *14* **MAX** *16*

SPIKES OK ? *Y*

This prompt asks for the spike (**SPK**) concentration and the expected **MIN**imum and **MAX**imum recovery (in concentration units) for each of the spikes for each analyte.

SO4 **DIFF IN DUPS** *1*
CL **DIFF IN DUPS** *2*

DIFF FOR DUPS OK? *Y*

The input required for this prompt is the allowable difference (in concentration units) between the "original" sample and its duplicate for each analyte.

TYPE OR GENERATE IDS (T OR G) ? *G*

Sample IDs are entered with this prompt. In addition, dilution factors (although not obvious by the prompt) are also specified. The prompt offers the operator two optional modes for entering these data. A *T* response means the operator must *T*ype each sample ID individually; a *G* response means the operator can *G*enerate a series of sample IDs by specifying the first and last ID in the series. The *T* response will be discussed later (see p. 21). The *G* response shown above produces the following prompt (operator responses are also shown):

********** SAMPLE WHEEL PATTERN **********

WHEEL PATTERN NO. 1 TIME: 8 : 45 DATE 6 / 26 / 1980

OPERATOR: FDS INSTRUMENT: TECHNICON AUTOANALYZER

STANDARDS SOURCE: FAKE INSTRUMENT CONDITIONS: OK

STUDY GROUP OR TITLE DEMONSTRATION

JCP	BLK	CS	SAMP	SPK	SAMP	DUP
	2	1	5	1	5	1

SAMPLES PER HOUR: 30

CHANNEL	A/D NO.	APPROX. LEVEL	BLANK DRIFT	UNITS	DATA RATE PTS/MIN	PEAK WIDTH	PLACES PAST DEC	ALLOWABLE NOISE, %FS
SO4	1	LO	2	PPM	30	N	1	2
CL	2	HI	3	PPM	35	B	1	2

RECORD	POS	NUMBER	TYPE	DIL	CONCENTRATIONS SO4	CL
1	1 1		SET			
2	1 2		SET			
3	1 3		SET			
4	1 4		BLK			
5	1 5		BLK			
6	1 6	S 1	STD		5.00	10.00
7	1 7	S 2	STD		10.00	20.00
8	1 8	S 3	STD		15.00	30.00
9	1 9	S 4	STD		20.00	50.00
10	1 10		BLK			
11	1 11		BLK			
12	1 12	CS 1	CS		5.00	20.00
13	1 13	101	SAMP	1		
14	1 14	102	SAMP	1		
15	1 15	103	SAMP	1		
16	1 16	104	SAMP	1		
17	1 17	105 R	RBL	1	ASSOC NOS. 101 TO 120	
18	1 18	101	SPK	1	5.00	15.00
19	1 19	106	SAMP	1		
20	1 20	109	SAMP	1		
21	1 21	110	SAMP	1		
22	1 22	111	SAMP	1		
23	1 23	112	SAMP	1		
24	1 24	108	DUP	1		
25	1 25		BLK			
26	1 26		BLK			

FIG. 5. Sample-wheel-pattern printout.

RECORD	POS	NUMBER	TYPE	DIL	CONCENTRATIONS SO4	CL
27	1 27	CS 1	CS		5.00	20.00
28	1 28	113	SAMP	1		
29	1 29	114	SAMP	1		
30	1 30	115	SAMP	1		
31	1 31	116	SAMP	1		
32	1 32	117	SAMP	1		
33	1 33	113	SPK	1	5.00	15.00
34	1 34	118	SAMP	1		
35	1 35	119	SAMP	1		
36	1 36	120	SAMP	1		
37	1 37	121	SAMP	2		
38	1 38	122	SAMP	2		
39	1 39	118	DUP	1		
40	1 40		BLK			
41	2 1		BLK			
42	2 2	CS 1	CS		5.00	20.00
43	2 3	123	SAMP	2		
44	2 4	125 R	RBL	2	ASSOC NOS. 102 TO 130	
45	2 5	126	SAMP	2		
46	2 6	127	SAMP	2		
47	2 7	128	SAMP	2		
48	2 8	123	SPK	2	5.00	15.00
49	2 9	129	SAMP	2		
50	2 10	130	SAMP	2		
51	2 11	131	SAMP	1		
52	2 12	132	SAMP	1		
53	2 13	133	SAMP	1		
54	2 14	129	DUP	2		
55	2 15		BLK			
56	2 16		BLK			
57	2 17	CS 1	CS		5.00	20.00
58	2 18	134	SAMP	1		
59	2 19	135 R	RBL	1	ASSOC NOS. 131 TO 140	
60	2 20	137	SAMP	1		
61	2 21	138	SAMP	1		
62	2 22	139	SAMP	1		
63	2 23	134	SPK	1	5.00	15.00
64	2 24	140	SAMP	1		
65	2 25	140	DUP	1		
66	2 26		BLK			
67	2 27		BLK			

FIG. 5. (Continued)

ENTER ID'S AND DIL FOR THE SET

1 ST NO.	LAST NO.	DIL
? *1Ø1*	? *12Ø*	? *1*
? *121*	? *13Ø*	? *2*
? *131*	? *14Ø*	? *1*
? *Ø*		

IDS AND DIL OK ? *Y*

Three sets are shown in the above example. Up to 2Ø sets may be generated and all samples in each set must have the same dilution factor. The dilution-factor value is the reciprocal of the number entered under DIL. Entering *1* means 1/1 of the original concentration or no dilution. A *2* would mean the sample has 1/2 the original concentration, and *1Ø* would be 1/1Ø of the original concentration, etc.

When a zero is entered for the ID (see above) it signals the computer that all information for IDs has been completed. Control then passes to the next item:

TYPE ALL MISSING SAMPLE NUMBERS

NO. 1Ø6
NO. 1Ø7
NO. 124
NO. 136
NO. Ø

NUMBERS OK ? *Y*

The generate-mode of entering sample numbers has been provided to minimize operator time for this task. If any sample IDs are missing for some reason (lost, spilled, or whatever) it is much easier for the operator to specify a series of numbers and then delete the numbers that are missing from that series. The computer program, when constructing the sample-wheel pattern, can then automatically exclude the missing IDs from the pattern. In the input example shown above, samples 1Ø6 and 1Ø7 are indicated as missing from the 1Ø1 to 12Ø series, sample 124 from the 121 to 13Ø series, and sample 136 from the 131 to 14Ø series. For the result in the sample-wheel pattern see Fig. 5.

Again, a zero as the last entry signifies the end of input for the prompt.

ENTER ALL RBL NOS. AND THE FIRST AND LAST SAMPLE NO. ASSOCIATED

RBL NO.	1 ST SAMP	LAST SAMP
? *1Ø5*	? *1Ø1*	? *12Ø*
? *125*	? *1Ø2*	? *13Ø*
? *135*	? *131*	? *14Ø*
? *Ø*		

RBLS OK ? *Y*

In some analyte determinations, a blank of the reagents (RBL) will be significant and thus a correction for the reagent blank must be made to the final analytical result. This prompt is provided to allow this to be done.

It must be kept in mind that, because RBLs are considered as samples when the QC pattern is being constructed by the computer, all RBLs must be assigned sample numbers. It is in responding to this prompt that the operator assigns a sample number to the RBL (under the heading **RBL NO.**). Examination of Fig. 5 reveals that RBL 1Ø5 (RECORD #17) has become the fifth sample in QC pattern #1. Under the next two columns **1 ST SAMP** and **LAST SAMP** are typed the first and last sample numbers in the series associated with the reagent blank. These are the samples to which the correction may be applied. Up to four blocks of samples may be associated with one reagent blank.

NO. OF CALIB STD ? *4*

ENTER CONC OF STDS

SO4	**S 1**	? *5*	**S 2**	? *1Ø*	**S 3**	? *15*	**S 4**	? *2Ø*
CL	**S 1**	? *1Ø*	**S 2**	? *2Ø*	**S 3**	? *3Ø*	**S 4**	? *5Ø*

STDS OK ? *Y*

Data for the calibration standards used in the calibrate pattern are now entered. Four standards will be used. The concentrations of the standards for each analyte are typed after each ? prompt.

On completion of the above inputs, a group of messages appears on the terminal:

WRITING FILES

1 PATTERNS COMPLETED
2 PATTERNS COMPLETED
3 PATTERNS COMPLETED
67 FILES IN THIS SET UP
67 ID FILES IN USE

The first message informs the operator that the input data is being written into files.

The next three indicate that three QC patterns have been completed. The last QC pattern (see Fig. 5) is not a complete pattern and therefore is not indicated as a completed pattern. The sample-wheel pattern contains 67 records and all 67 will be processed.

(TAAIN chains to TAAINRE at this point. No indication of this is given.)

HEADER INFO ? *Y*

This prompt allows the operator to enter important information that will be printed on reports. In addition, the time and date generated by the computer are recorded and will also appear on the reports.

An examination of the following prompts and responses explains the type of information required:

OPERATOR *FBS*
INSTRUMENT CONDITIONS *OK*
STUDY OR GROUP TITLE *TEST 1*
STANDARDS SOURCE *FAKE DATA-DEMONSTRATION*

Note: Commas are not allowed in header information.

The next prompts ask if the operator wishes to edit the sample-wheel pattern and whether a printout of it is wanted.

EDIT FILES ? *N*
PRINT FILES ? *Y*

The EDIT response is *NO* because a printout has not yet been made; a *YES* response to **PRINT FILES** provides a printout.

On examination of the sample-wheel pattern (Fig. 5) an error is revealed in record number 44, namely, that the first sample number associated with RBL 125 R is shown as 1Ø2 instead of 121. The operator had made a mistake when entering the data in response to **ENTER ALL RBL NOS.** etc. (See section on p. 18).

EDIT FILES ? *Y*
RECORD NO. *44*

The operator can now correct this error by responding *YES* to the EDIT prompt, and then supplying the appropriate RECORD NO., which in this example is *44*. Seven column headings are then displayed on the terminal, followed by a line showing the analyte and solution type, along with the presently stored data for that analyte. A third line is a series of question marks under each datum:

CONST	TYPE	NO.	DIL	CONC	S1	S2
SO4	RBL	125	2	1	1Ø2	13Ø
		? 125	*? 2*	*? 1*	*? 121*	*? 13Ø*
CL	RBL	125	2	1	1Ø2	13Ø
		? 125	*? 2*	*? 1*	*? 121*	*? 13Ø*

If the value above each question mark is valid, it is retyped; if not, the correct value is typed. This is done for each analyte. (Note: The 1 under CONC indicates that there is only one series of samples associated with this reagent blank. S1 and S2 refer to the first and last samples associated with the RBL.) When more than one series of samples is associated with a given RBL, *only the first set is accessible using the EDIT option.*

After the correct data have been entered, the next prompt asks for the next record number to be edited;

RECORD NO. *Ø*

If none, respond with a zero.

PRINT FILES ? *Y*
EDIT FILES ? *N*

The edited sample-wheel pattern is printed (see Fig. 5) and found to be correct. If incorrect, the editing process can be repeated. A *NO* response to **EDIT FILES ?** produces the following:

ADDITIONS OR DELETIONS ? *N*

A *YES* response allows addition or deletion of samples. See section on editing below for more detailed treatment.

ANY OTHER CHANGES ? *N*

This is also covered in the section on editing (below) and refers to editing changes requiring corrections to items not covered by TAAINRE.

This is the last of the prompts for entering data. The following terminal message now appears.

TAASTART 2809 05/24/77 13:20 800 DC

This message informs the operator that all input data have been stored and that TAASTART has been chained to begin analytical data taking. See section on calibration and analysis for operating details of TAASTART.

Note on the use of the *T* option.

We considered above the use of the *G* (*G*enerate) option for entering sample ID data (see p. 15). The alternate option *T* (*T*ype) is used when entering sample ID data for each individual sample one at a time. This mode is used most advantageously where a small number of samples that are known to require various dilution factors must be entered.

Figure 6 is a portion of the actual prompts and responses for another set of samples (no relationship to the previous example) to illustrate the sequence of prompts after requesting the *T* option. It can be seen that the sample ID data are not entered immediately, as with the *G* option, but only after the **RBL** and **CALIB STDS** data have been typed, and after the **WRITING FILES** message.

In this example the QC pattern does not have any samples associated with spikes and only 5 samples with 1 duplicate. When entering the sample IDs singly, each time a QC pattern is filled (5 samples in this case) a computer message informs the operator of this fact. A comparison of Figs. 4 and 6 will make clear the difference in the data-input sequence between the *T* and *G* options.

ENTERING DATA FOR A CONTINUING RUN OR A NORMAL RUN

Continuing Run

A continuing run assumes that data for a new run have been entered as previously described. Only the additional sample IDs for the same batch of samples need be entered. When the prompt **DO YOU WANT**

```
QCP        BLK        CS         SAMP       SPK        SAMP       DUP
           ? 2        ? 1        ? Ø        ? Ø        ? 5        ? 1

PATTERN OK ? Y

SO4        CS 1   ? 5    ERR 1
CL         CS 1   ? 2Ø   ERR 2

CHECK STDS OK Y

SO4        DIFF IN DUPS 1
CL         DIFF IN DUPS 2

DIFF FOR DUPS OK Y

TYPE OR GENERATE IDS (T OR G) ? T

ENTER ALL RBL NOS. AND THE FIRST AND LAST SAMPLE NO. ASSOCIATED

  RBL NO.          1 ST SAMP          LAST SAMP
  ? 1Ø5              ? 1Ø1              ? 112
  ? Ø

RBLS OK ? Y

NO. OF CALIB STDS ? 4

ENTER CONC OF STDS

SO4        S 1   ? 5    S 2   ? 1Ø   S 3   ? 15   S 4   ? 2Ø
CL         S 1   ? 1Ø   S 2   ? 2Ø   S 3   ? 3Ø   S 4   ? 5Ø

STDS OK ? Y
```

FIG. 6. Operator dialogue for QC pattern—use of T-option.

```
WRITING FILES
ID 101      DIL 1
ID 102      DIL 10
ID 103      DIL 1
ID 104      DIL 5
ID 105      DIL 1

 1  PATTERNS COMPLETED

ID 108      DIL 40
ID 109      DIL 10
ID 110      DIL 1
ID 111      DIL 5
ID 112      DIL 1

 2  PATTERNS COMPLETED
ID  0  32  FILES IN THIS SET UP
  32  ID FILES IN USE

HEADER INFO ? Y
OPERATOR     FBS
INSTRUMENT CONDITIONS     OK
STUDY OR GROUP TITLE     TEST2
STANDARDS SOURCE     FAKE
EDIT FILES ? N
PRINT FILES ? Y
EDIT FILES ? N
ADDITIONS OR DELETIONS ? N
ANY OTHER CHANGES ? N
TAASTART 2809 05/24/77 13:20 800 DC
```

FIG. 6. (cont.)

TO ENTER NEW DATA... appears on the terminal, the proper resonse is *N*ONE because no new data (other than the sample IDs) are required. Figure 7 shows the prompts and responses for this type of run and Fig. 8 shows the resulting sample-wheel pattern.

```
*RUN"TAAIN
DO YOU WANT TO RUN PREVIOUSLY STORED SAMPLE ID NOS. ? N
WHEEL PATTERN NO. (1 TO 9) 2
IS THIS A RE-START OF AN INTERRUPTED RUN ? N
DO YOU WANT TO ENTER NEW DATA
FOR EACH CHAN., QC PATT., STND. CONC., QC LIMITS
ANSWER ALL, SOME, OR NONE (A,S,N) ? N
RUN NUMBER          2
 67      ID FILES IN LAST RUN
TYPE OR GENERATE IDS (T OR G) ? G

ENTER ID'S AND DIL FOR THE SET

1 ST NO.            LAST NO.            DIL
  ? 200               ? 219               ? 1
  ? 220               ? 229               ? 10
  ? 230               ? 249               ? 5
  ? 0

IDS AND DIL OK ? Y

TYPE ALL MISSING SAMPLE NUMBERS

NO.    209
NO.    0

NUMBERS OK ? Y

ENTER ALL RBL NOS. AND THE FIRST AND LAST SAMPLE NO. ASSOCIATED

RBL NO.             1ST SAMP            LAST SAMP
? 0

RBLS OK ? Y
```

FIG. 7. Operator dialogue when using stored data.

```
SO4                    CL

1       PATTERNS COMPLETED
2       PATTERNS COMPLETED
3       PATTERNS COMPLETED
4       PATTERNS COMPLETED
5       PATTERNS COMPLETED
85      FILES IN THIS SET UP
385     ID FILES IN USE
HEADER INFO ? N
EDIT FILES ? N
PRINT FILES ? Y
EDIT FILES ? N
ADDITIONS OR DELETIONS ? N
ANY OTHER CHANGES ? N
TAASTART 2809 05/24/77 13:20 800 DC

STOP AT 0010
.
```

FIG. 7. (cont.)

Normal Run

In an established laboratory it can normally be expected that different sample batches will require some new data (other than sample IDs) to be entered. For example, the range of the calibration standards may need to be changed, or the use of spiked samples may be required. For entering new data such as these, the proper response to the prompt **DO YOU WANT TO ENTER NEW DATA...** is *S*OME. This option allows changes to be made in several parameters. Figure 9 shows the prompts and responses for the same sample IDs as the previous continuing run examples. Here, however, the operator required a change in the check standards concentrations. Some other parameters could have been altered if desired. Figure 10 shows the resulting sample-wheel pattern with the new check standard concentration.

EDITING

The EDIT Option

The prompt:

```
EDIT FILES ? Y
```

with a *Y*ES response as shown above, allows the operator to change numbers that have already been entered. This EDIT feature allows *only data that are associated with a RECORD number to be changed.* All record numbers, wheel numbers, positions, solution IDs, solution types, and dilution factors are stored in a temporary file called TAAID. (All other information, such as reader information, data rates, peak width, etc., are stored in a permanent file called TAAINF.) Editing can be done either before or after printing the sample-wheel pattern; the usual practice, however, is to edit after examining the printout.

********** SAMPLE WHEEL PATTERN **********

WHEEL PATTERN NO. 2 TIME: 8 : 51 DATE 6 / 26 / 1980

OPERATOR: FBS INSTRUMENT: TECHNICON AUTOANALYZER

STANDARDS SOURCE: FAKE INSTRUMENT CONDITIONS: OK

STUDY GROUP OR TITLE DEMONSTRATION

UCP	BLK	CS	SAMP	SPK	SAMP	DUP
	2	1	5	1	5	1

SAMPLES PER HOUR: 30

CHANNEL	A/D NO.	APPROX. LEVEL	BLANK DRIFT	UNITS	DATA RATE PTS/MIN	PEAK WIDTH	PLACES PAST DEC	ALLOWABLE NOISE, %FS
SO4	1	LO	2	PPM	30	N	1	2
CL	2	HI	3	PPM	35	B	1	2

RECORD	POS		NUMBER	TYPE	DIL	CONCENTRATIONS SO4	CL
501	1	1		SET			
502	1	2		SET			
503	1	3		SET			
504	1	4		BLK			
505	1	5		BLK			
506	1	6	S 1	STD		5.00	10.00
507	1	7	S 2	STD		10.00	20.00
508	1	8	S 3	STD		15.00	30.00
509	1	9	S 4	STD		20.00	50.00
510	1	10		BLK			
511	1	11		BLK			
512	1	12	CS 1	CS		5.00	20.00
513	1	13	200	SAMP	1		
514	1	14	201	SAMP	1		
515	1	15	202	SAMP	1		
516	1	16	203	SAMP	1		
517	1	17	204	SAMP	1		
518	1	18	200	SPK	1	5.00	15.00
519	1	19	205	SAMP	1		
520	1	20	206	SAMP	1		
521	1	21	207	SAMP	1		
522	1	22	208	SAMP	1		
523	1	23	210	SAMP	1		
524	1	24	205	DUP	1		
525	1	25		BLK			
526	1	26		BLK			
527	1	27	CS 1	CS		5.00	20.00
528	1	28	211	SAMP	1		
529	1	29	212	SAMP	1		
530	1	30	213	SAMP	1		
531	1	31	214	SAMP	1		
532	1	32	215	SAMP	1		
533	1	33	211	SPK	1	5.00	15.00

FIG. 8. Sample-wheel-pattern printout using stored data.

RECORD		POS	NUMBER	TYPE	DIL	CONCENTRATIONS SO4	CL
534	1	34	216	SAMP	1		
535	1	35	217	SAMP	1		
536	1	36	218	SAMP	1		
537	1	37	219	SAMP	1		
538	1	38	220	SAMP	10		
539	1	39	216	DUP	1		
540	1	40		BLK			
541	2	1		BLK			
542	2	2	CS 1	CS		5.00	20.00
543	2	3	221	SAMP	10		
544	2	4	222	SAMP	10		
545	2	5	223	SAMP	10		
546	2	6	224	SAMP	10		
547	2	7	225	SAMP	10		
548	2	8	221	SPK	10	5.00	15.00
549	2	9	226	SAMP	10		
550	2	10	227	SAMP	10		
551	2	11	228	SAMP	10		
552	2	12	229	SAMP	10		
553	2	13	230	SAMP	5		
554	2	14	226	DUP	10		
555	2	15		BLK			
556	2	16		BLK			
557	2	17	CS 1	CS		5.00	20.00
558	2	18	231	SAMP	5		
559	2	19	232	SAMP	5		
560	2	20	233	SAMP	5		
561	2	21	234	SAMP	5		
562	2	22	235	SAMP	5		
563	2	23	231	SPK	5	5.00	15.00
564	2	24	236	SAMP	5		
565	2	25	237	SAMP	5		
566	2	26	238	SAMP	5		
567	2	27	239	SAMP	5		
568	2	28	240	SAMP	5		
569	2	29	236	DUP	5		
570	2	30		BLK			
571	2	31		BLK			
572	2	32	CS 1	CS		5.00	20.00
573	2	33	241	SAMP	5		
574	2	34	242	SAMP	5		
575	2	35	243	SAMP	5		
576	2	36	244	SAMP	5		
577	2	37	245	SAMP	5		
578	2	38	241	SPK	5	5.00	15.00
579	2	39	246	SAMP	5		
580	2	40	247	SAMP	5		
581	3	1	248	SAMP	5		
582	3	2	249	SAMP	5		
583	3	3	246	DUP	5		
584	3	4		BLK			
585	3	5		BLK			

FIG. 8. (Continued)

```
*RUN"TAAIN
DO YOU WANT TO RUN PREVIOUSLY STORED SAMPLE ID NOS. ? N
WHEEL PATTERN NO. (1 TO 9) 4
IS THIS A RE-START OF AN INTERRUPTED RUN ? N
DO YOU WANT TO ENTER NEW DATA
FOR EACH CHAN., QC PATT., STND. CONC., QC LIMITS
ANSWER ALL, SOME, OR NONE (A,S,N) ? S
WHICH VARIABLES DO YOU WANT TO CHANGE (Y OR N) ?

QCP             CS              SPK             STDS            DUP DIFF
? N             ? Y             ? N             ? N             ? N

NUMBER OF SAMPLES PER HOUR ? 30

RUN NUMBER          3
 85    ID FILES IN LAST RUN

SO4          CS 1    ? 30    ERR .3
CL           CS 1    ? 35    ERR 1

CHECK STDS OK Y

TYPE OR GENERATE IDS (T OR G) ? G

ENTER ID'S AND DIL FOR THE SET

1ST NO.         LAST NO.        DIL
  ? 200           ? 219           ? 1
  ? 220           ? 229           ? 10
  ? 230           ? 249           ? 5
  ? 0

ID'S AND DIL OK ? Y

TYPE ALL MISSING SAMPLE NUMBERS

NO.    209
NO.    0

NUMBERS OK ? Y
```

FIG. 9. Operator dialogue when using some new data.

```
ENTER ALL RBL NOS. AND THE FIRST AND LAST SAMPLE NO. ASSOCIATED

RBL NO.              1ST SAMP              LAST SAMP
? Ø

RBLS OK ? Y

SO4                  CL

1       PATTERNS COMPLETED
2       PATTERNS COMPLETED
3       PATTERNS COMPLETED
4       PATTERNS COMPLETED
5       PATTERNS COMPLETED
85      FILES IN THIS SET UP
385     ID FILES IN USE
HEADER INFO ? N
EDIT FILES ? N
PRINT FILES ? Y
EDIT FILES ? N
ADDITIONS OR DELETIONS ? N
ANY OTHER CHANGES ? N
TAASTART 28Ø9 Ø5/24/77 13:2Ø 8ØØ DC

STOP AT ØØ7Ø
```

FIG. 9. (cont.)

Previously, on p. 20, a detailed example of editing was given, illustrating how to change the series of samples associated with RBLs. The format of the prompt headings:

CONST TYPE NO. DIL CONC S1 S2

is a generalized one that is used for making changes for all of the different types of solutions in the sample wheel. Some of the headings may have different meanings, depending on the solution type. Also, the value under a heading may or may not have significance with reference to a particular solution. For example, **CONC** has no significance in reference to a SAMPLE type solution, but it does for any type of standard or spike. When a heading has no significance, a zero appears under it.

The headings **S1** and **S2** are generalized headings. When editing for RBL changes, **S1** and **S2** refer to the beginning and ending sample numbers associated with the RBL. Also, for RBLs, a value appearing under the **CONC** heading refers to how many series of samples are associated with the RBL and has no reference to concentration!

********** SAMPLE WHEEL PATTERN **********

WHEEL PATTERN NO. 4 TIME: 8 : 58 DATE 6 / 26 / 1980

OPERATOR: FBS INSTRUMENT: TECHNICON AUTOANALYZER

STANDARDS SOURCE: FAKE INSTRUMENT CONDITIONS: OK

STUDY GROUP OR TITLE DEMONSTRATION

RCP	BLK	CS	SAMP	SPK	SAMP	DUP
	2	1	5	1	5	1

SAMPLES PER HOUR: 30

CHANNEL	A/D NO.	APPROX. LEVEL	BLANK DRIFT	UNITS	DATA RATE PTS/MIN	PEAK WIDTH	PLACES PAST DEC	ALLOWABLE NOISE, %FS
SO4	1	LO	2	PPM	30	N	1	2
CL	2	HI	3	PPM	35	N	1	2

RECORD	POS		NUMBER	TYPE	DIL	CONCENTRATIONS SO4	CL
901	1	1		SET			
902	1	2		SET			
903	1	3		SET			
904	1	4		BLK			
905	1	5		BLK			
906	1	6	S 1	STD		5.00	10.00
907	1	7	S 2	STD		10.00	20.00
908	1	8	S 3	STD		15.00	30.00
909	1	9	S 4	STD		20.00	50.00
910	1	10		BLK			
911	1	11		BLK			
912	1	12	CS 1	CS		30.00	35.00
913	1	13	200	SAMP	1		
914	1	14	201	SAMP	1		
915	1	15	202	SAMP	1		
916	1	16	203	SAMP	1		
917	1	17	204	SAMP	1		
918	1	18	200	SPK	1	5.00	15.00
919	1	19	205	SAMP	1		
920	1	20	206	SAMP	1		
921	1	21	207	SAMP	1		
922	1	22	208	SAMP	1		
923	1	23	210	SAMP	1		
924	1	24	205	DUP	1		
925	1	25		BLK			
926	1	26		BLK			
927	1	27	CS 1	CS		30.00	35.00
928	1	28	211	SAMP	1		
929	1	29	212	SAMP	1		
930	1	30	213	SAMP	1		
931	1	31	214	SAMP	1		

FIG. 10. Sample-wheel-pattern printout resulting from run shown in Fig. 9.

RECORD	POS		NUMBER	TYPE	DIL	CONCENTRATIONS SO4	CL
932	1	32	215	SAMP	1		
933	1	33	211	SPK	1	5.00	15.00
934	1	34	216	SAMP	1		
935	1	35	217	SAMP	1		
936	1	36	218	SAMP	1		
937	1	37	219	SAMP	1		
938	1	38	220	SAMP	10		
939	1	39	216	DUP	1		
940	1	40		BLK			
941	2	1		BLK			
942	2	2	CS 1	CS		30.00	35.00
943	2	3	221	SAMP	10		
944	2	4	222	SAMP	10		
945	2	5	223	SAMP	10		
946	2	6	224	SAMP	10		
947	2	7	225	SAMP	10		
948	2	8	221	SPK	10	5.00	15.00
949	2	9	226	SAMP	10		
950	2	10	227	SAMP	10		
951	2	11	228	SAMP	10		
952	2	12	229	SAMP	10		
953	2	13	230	SAMP	5		
954	2	14	226	DUP	10		
955	2	15		BLK			
956	2	16		BLK			
957	2	17	CS 1	CS		30.00	35.00
958	2	18	231	SAMP	5		
959	2	19	232	SAMP	5		
960	2	20	233	SAMP	5		
961	2	21	234	SAMP	5		
962	2	22	235	SAMP	5		
963	2	23	231	SPK	5	5.00	15.00
964	2	24	236	SAMP	5		
965	2	25	237	SAMP	5		
966	2	26	238	SAMP	5		
967	2	27	239	SAMP	5		
968	2	28	240	SAMP	5		
969	2	29	236	DUP	5		
970	2	30		BLK			
971	2	31		BLK			
972	2	32	CS 1	CS		30.00	35.00
973	2	33	241	SAMP	5		
974	2	34	242	SAMP	5		
975	2	35	243	SAMP	5		
976	2	36	244	SAMP	5		
977	2	37	245	SAMP	5		
978	2	38	241	SPK	5	5.00	15.00
979	2	39	246	SAMP	5		
980	2	40	247	SAMP	5		
981	3	1	248	SAMP	5		
982	3	2	249	SAMP	5		
983	3	3	246	DUP	5		
984	3	4		BLK			
985	3	5		BLK			

FIG. 10. (Continued)

For spike (SPK) solutions, **S1** refers to the RECORD NO. for the appropriate sample number under **NO.**; **S2** refers to the consecutive number of the spike in the QC pattern.

The second line of the prompt shows the constituent and the sample type followed by the values for each parameter heading presently stored. The third line of the prompt is a series of question marks. If the presently stored value is valid it is retyped; if not, a new value is entered. Some editing examples follow:

- Changing a sample dilution factor.

PRINT FILES ? *Y*
EDIT FILES ? *Y*
RECORD NO. *636*

CONST	TYPE	NO.	DIL	CONC	S1	S2
SO4	SAMPLE	12Ø	.1	Ø	Ø	Ø
		? 12Ø	*? 1Ø*	*? Ø*	*? Ø*	*? Ø*
CL	SAMPLE	12Ø	1	Ø	Ø	Ø
		? 12Ø	*? 1Ø*	*? Ø*	*? Ø*	*? Ø*

Comment: Notice that the edited change has to be made for all analytes being run.

- Changing the sample to be duplicated.

RECORD NO. *639*

CONST	TYPE	NO.	DIL	CONC	S1	S2
SO4	DUP	118	1	Ø	634	Ø
		? 12Ø	*? 1Ø*	*? Ø*	*? 636*	*? Ø*
CL	DUP	118	1	Ø	634	Ø
		? 12Ø	*? 1Ø*	*? Ø*	*? 636*	*? Ø*

Comment: The sample ID to be duplicated is being changed from 118 (RECORD NO. 634) to 12Ø (RECORD NO. 636). Both the sample ID *and* the RECORD NO. must be changed. Note also that the DILution factor has also been changed to agree with the dilution change made above for RECORD NO. 636.

- Changing the concentration of a check standard (or calibration standard).

RECORD NO. *627*

CONST	TYPE	NO.	DIL	CONC	S1	S2
SO4	CS	1	1	5	Ø	Ø
		? 1	*? 1*	*? 1Ø*	*? Ø*	*? Ø*
CL	CS	1	1	2Ø	Ø	Ø
		? 1	*? 1*	*? 25*	*? Ø*	*? Ø*

Comment: Check Standard No. 1 requires no change in DILution factor, but the CONCentration for both analytes has been changed.

- Changing the sample to be spiked.

RECORD NO. *618*

CONST	TYPE	NO.	DIL	CONC	S1	S2
SO4	SPK	1Ø1	1	5	613	1
		? *1Ø4*	? *1*	? *5*	? *616*	? *1*
CL	SPK	1Ø1	1	15	613	1
		? *1Ø4*	? *1*	? *15*	? *616*	? *1*

Comment: The sample ID to be spiked is being changed from 1Ø1 (RECORD NO. 613) to 1Ø4 (RECORD NO. 616). No change in DILution factor is required nor is a change in spike CONCentration being made. The value **1** under heading **S2** means that this is the first spiked sample in the QCP. Had this been the second spiked sample, a **2** would have appeared under **S2**. Special care must be taken when making editing changes for spikes and duplicates to see that all common parameters agree with those of the sample being spiked or duplicated.

- Terminating the EDIT function.

RECORD NO. *Ø*

Comment: Typing a zero after the prompt terminates editing.

PRINT FILES ? *Y*
EDIT FILES ? *N*
ADDITIONS OR DELETIONS ? *N*
ANY OTHER CHANGES ? *N*
TAASTART 28Ø9 Ø5/24/77 13:2Ø 8ØØ DC

- Figures 11a and 11b are partial printouts of a sample-wheel pattern, which allow a before and after comparison to be made of all the editing changes just illustrated above.

Additions and Deletions

Additional samples can be added to the sample-wheel pattern, and samples can be deleted from those already in the pattern. A *Yes* response allows the operator to add samples, delete samples, or to do both. A *No* response indicates neither will be done.

Additions are always requested first and, if any, are always added to the last QC pattern of the sample-wheel pattern.

ADDITIONS OR DELETIONS ? *Y*
ADDITIONS, Ø TO END
ID *141* **DIL** *1*

********** SAMPLE WHEEL PATTERN **********

WHEEL PATTERN NO. 3 TIME: 9 : 7 DATE 6 / 26 / 1980

OPERATOR: FBS INSTRUMENT: TECHNICON AUTOANALYZER

STANDARDS SOURCE: FAKE INSTRUMENT CONDITIONS: OK

STUDY GROUP OR TITLE DEMONSTRATION

JCP	BLK	CS	SAMP	SPK	SAMP	DUP
	2	1	5	1	5	1

SAMPLES PER HOUR: 30

CHANNEL	A/D NO.	APPROX. LEVEL	BLANK DRIFT	UNITS	DATA RATE PTS/MIN	PEAK WIDTH	PLACES PAST DEC	ALLOWABLE NOISE, %FS
SO4	1	LO	2	PPM	30	N	1	2
CL	2	HI	3	PPM	35	B	1	2

RECORD	POS	NUMBER	TYPE	DIL	CONCENTRATIONS SO4	CL
601	1 1		SET			
602	1 2		SET			
603	1 3		SET			
604	1 4		BLK			
605	1 5		BLK			
606	1 6	S 1	STD		5.00	10.00
607	1 7	S 2	STD		10.00	20.00
608	1 8	S 3	STD		15.00	30.00
609	1 9	S 4	STD		20.00	50.00
610	1 10		BLK			
611	1 11		BLK			
612	1 12	CS 1	CS		30.00	35.00
613	1 13	101	SAMP	1		
614	1 14	102	SAMP	1		
615	1 15	103	SAMP	1		
616	1 16	104	SAMP	1		
617	1 17	105 R	R&L	1	ASSOC NOS. 101 TO 120	
618	1 18	104	SPK	1	5.00	15.00
619	1 19	108	SAMP	1		
620	1 20	109	SAMP	1		
621	1 21	110	SAMP	1		
622	1 22	111	SAMP	1		
623	1 23	112	SAMP	1		
624	1 24	108	DUP	1		
625	1 25		BLK			
626	1 26		BLK			

FIG. 11a. Printout of sample-wheel-pattern before editing.

RECORD		POS	NUMBER	TYPE	DIL	CONCENTRATIONS SO4	CL
627	1	27	CS 1	CS		10.00	25.00
628	1	28	113	SAMP	1		
629	1	29	114	SAMP	1		
630	1	30	115	SAMP	1		
631	1	31	116	SAMP	1		
632	1	32	117	SAMP	1		
633	1	33	113	SPK	1	5.00	15.00
634	1	34	118	SAMP	1		
635	1	35	119	SAMP	1		
636	1	36	120	SAMP	10		
637	1	37	121	SAMP	2		
638	1	38	122	SAMP	2		
639	1	39	120	DUP	10		
640	1	40		BLK			
641	2	1		BLK			
642	2	2	CS 1	CS		30.00	35.00
643	2	3	123	SAMP	2		
644	2	4	125 R	RBL	2	ASSOC NOS. 121 TO 130	
645	2	5	126	SAMP	2		
646	2	6	127	SAMP	2		
647	2	7	128	SAMP	2		
648	2	8	123	SPK	2	5.00	15.00
649	2	9	129	SAMP	2		
650	2	10	130	SAMP	2		
651	2	11	131	SAMP	1		
652	2	12	132	SAMP	1		
653	2	13	133	SAMP	1		
654	2	14	129	DUP	2		
655	2	15		BLK			
656	2	16		BLK			
657	2	17	CS 1	CS		30.00	35.00
658	2	18	134	SAMP	1		
659	2	19	135 R	RBL	1	ASSOC NOS. 131 TO 140	
660	2	20	137	SAMP	1		
661	2	21	138	SAMP	1		
662	2	22	139	SAMP	1		
663	2	23	134	SPK	1	5.00	15.00
664	2	24	140	SAMP	1		
665	2	25	140	DUP	1		
666	2	26		BLK			
667	2	27		BLK			

FIG. 11a. (Continued)

********** SAMPLE WHEEL PATTERN **********

WHEEL PATTERN NO. 3 TIME: 9 : 7 DATE 6 / 26 / 1980

OPERATOR: FBS INSTRUMENT: TECHNICON AUTOANALYZER

STANDARDS SOURCE: FAKE INSTRUMENT CONDITIONS: OK

STUDY GROUP OR TITLE DEMONSTRATION

QCP	BLK	CS	SAMP	SPK	SAMP	DUP
	2	1	5	1	5	1

SAMPLES PER HOUR: 30

CHANNEL	A/D NO.	APPROX. LEVEL	BLANK DRIFT	UNITS	DATA RATE PTS/MIN	PEAK WIDTH	PLACES PAST DEC	ALLOWABLE NOISE, %FS
SO4	1	LO	2	PPM	30	N	1	2
CL	2	HI	3	PPM	35	B	1	2

RECORD	POS	NUMBER	TYPE	DIL	CONCENTRATIONS SO4	CL
601	1 1		SET			
602	1 2		SET			
603	1 3		SET			
604	1 4		BLK			
605	1 5		BLK			
606	1 6	S 1	STD		5.00	10.00
607	1 7	S 2	STD		10.00	20.00
608	1 8	S 3	STD		15.00	30.00
609	1 9	S 4	STD		20.00	50.00
610	1 10		BLK			
611	1 11		BLK			
612	1 12	CS 1	CS		30.00	35.00
613	1 13	101	SAMP	1		
614	1 14	102	SAMP	1		
615	1 15	103	SAMP	1		
616	1 16	104	SAMP	1		
617	1 17	105 R	RBL	1	ASSOC NOS. 101 TO 120	
618	1 18	101	SPK	1	5.00	15.00
619	1 19	108	SAMP	1		
620	1 20	109	SAMP	1		
621	1 21	110	SAMP	1		
622	1 22	111	SAMP	1		
623	1 23	112	SAMP	1		
624	1 24	106	DUP	1		
625	1 25		BLK			
626	1 26		BLK			

FIG. 11b. Printout of sample-wheel-pattern after editing.

RECORD	POS		NUMBER	TYPE	DIL	CONCENTRATIONS SO4	CL
627	1	27	CS 1	CS		5.00	20.00
628	1	28	113	SAMP	1		
629	1	29	114	SAMP	1		
630	1	30	115	SAMP	1		
631	1	31	116	SAMP	1		
632	1	32	117	SAMP	1		
633	1	33	113	SPK	1	5.00	15.00
634	1	34	118	SAMP	1		
635	1	35	119	SAMP	1		
636	1	36	120	SAMP	1		
637	1	37	121	SAMP	2		
638	1	38	122	SAMP	2		
639	1	39	118	DUP	1		
640	1	40		BLK			
641	2	1		BLK			
642	2	2	CS 1	CS		30.00	35.00
643	2	3	123	SAMP	2		
644	2	4	125 R	RBL	2	ASSOC NOS. 121 TO 130	
645	2	5	126	SAMP	2		
646	2	6	127	SAMP	2		
647	2	7	128	SAMP	2		
648	2	8	123	SPK	2	5.00	15.00
649	2	9	129	SAMP	2		
650	2	10	130	SAMP	2		
651	2	11	131	SAMP	1		
652	2	12	132	SAMP	1		
653	2	13	133	SAMP	1		
654	2	14	129	DUP	2		
655	2	15		BLK			
656	2	16		BLK			
657	2	17	CS 1	CS		30.00	35.00
658	2	18	134	SAMP	1		
659	2	19	135 R	RBL	1	ASSOC NOS. 131 TO 140	
660	2	20	137	SAMP	1		
661	2	21	138	SAMP	1		
662	2	22	139	SAMP	1		
663	2	23	134	SPK	1	5.00	15.00
664	2	24	140	SAMP	1		
665	2	25	140	DUP	1		
666	2	26		BLK			
667	2	27		BLK			

FIG. 11b. (Continued)

ID *142* **DIL** *1ø*
ID *ø*

The prompt asks for sample IDs and DILution factors. It also reminds the operator that ø (zero) terminates the addition of samples. After termination, the next prompt asks for deletions.

DELETIONS, ø TO END
RECORD NO. *63ø*
WANT TO DELETE SAMPLE NO. 115 ? *Y*

When deleting a sample, two prompts must be answered: first the record number, and then a confirmation using the sample number. This double check is done to minimize the accidental deletion of the wrong sample. Once deleted, the sample can no longer be replaced into the same location in the pattern because, as pointed out above, added samples always go into the last QC pattern.

Only samples may be deleted. It does not matter whether the sample appears later in the pattern as a duplicate or a spiked sample. A duplicate by itself, or a spiked sample by itself, cannot be deleted. Attempts to delete any solution other than a SAMPLE will prompt an error message as in the following example:

RECORD NO. *627*
BAD RECORD NO., NOT A SAMPLE
RECORD NO. *ø*

In the above, RECORD No. 627 was a check standard.

When the next request for a record number appears, a record number corresponding to a sample can be typed, or a zero indicating the deletions are complete. A new sample-wheel pattern can now be generated and printed.

Other Changes

Thus far, editing has been performed only on sample-wheel-pattern data (TAAID file). To make other changes, accessing the permanent file TAAINF will be necessary. If *Y*es is the response to the prompt:

ANY OTHER CHANGES ? *Y*

a restart is automatically made and TAAIN is chained in. This means that the operator must reply *N*O to the prompts **DO YOU WANT TO RUN PREVIOUSLY STORED SAMPLE ID NOS.?** and **IS THIS A RESTART OF AN INTERRUPTED RUN?**. It will also be necessary to respond *A*LL to the prompt **DO YOU WANT TO ENTER NEW DATA....** The *A*LL response will allow the operator to increase the number of spikes and check standards (and their concentrations) in the QC pattern, and the number of calibration standards and their concentrations in the calibrate pattern. However, to decrease the number of spikes and/or check standards in the QC pattern, the *S*OME option may be used. In either case, all of the data called for by the respective prompts will have to be reentered, including all sample ID data.

If, when using the *S*OME option, an operator attempts to increase the number of check standards or spikes to a higher value than that already stored, error messages will appear on the terminal, for example,

NOT ENOUGH SPIKES IN FILE or **NOT ENOUGH CHECK STDS IN FILE.**

If this occurs, the operator will have to limit the run to the number of spikes and check standards in file or make changes using one of the options described above.

LINE PRINTER OUTPUT

The line printer is an important output device in the system. Since many operators may require use of the printer at the same time, it is possible for conflicts to occur. If they do, the following message will appear:

LINEPRINTER IN USE, WILL RETRY EVERY 1Ø SECS. FOR 2 MINS.

If after two minutes there is still no response, this message appears:

LINEPRINTER STILL IN USE AFTER 2 MIN., TYPE CON TO KEEP TRYING STOP AT 3Ø6Ø.

Either you are very unlucky or there is something wrong with the computer. It is a good idea to contact your computer coordinator at this point.

CON

With luck, it will print now.

CALIBRATION AND ANALYSIS

SCOPE

Once all input data have been entered and the sample wheel(s) loaded with solutions in conformance with the sample-wheel pattern, a series of programs is used to initialize and calibrate the system, and to analyze samples. The programs are TAASTART, TAACAL, TAA, and TAAQCOP.

TAASTART is a short, simple program to confirm that the colorimeter output signal has the appropriate zero- to full-scale range, and to establish the timing that correlates a peak to the appropriate wheel-pattern location. It initiates a real-time assembly-language program to detect the peak heights of the set standards in the calibrate pattern.

TAACAL reads the peak heights for the calibration standards and the blanks on either side. It calculates the coefficients of the polynomial equations used in sample analysis to convert peak heights to concentration.

TAA reads the peak heights for all the solutions in the QC Pattern. This includes check standards, samples, reagent blanks, spiked samples, duplicates, and blanks. It provides on-line results for samples.

TAAQCOP provides QC warnings and on-line results for all solutions except samples.

For more detailed information refer to Volume 2, *Notes to Coordinator...*, and Volume 4, *Detailed Description...*, Parts 3, 4, and 5, of this report (UCRL-52532).

Initialization (TAASTART)

There are two ways to arrive at the program TAASTART. Normally, after setting up the sample-wheel pattern using the programs TAAIN/TAAINRE, TAASTART will run automatically. Alternatively, if a previously stored set of samples is to be run, the operator can type the command *RUN TAASTART*. This alternative method must be used with caution, however, because the sample-wheel pattern that will be processed will be the last one that was referenced under the ACCOUNT-ID used when last logging on. Perhaps the safest method is to run TAAIN, specify the sample-wheel number, and appropriately answer the few remaining questions.

Full-scale and Baseline Check

When TAASTART begins, two prompts are issued:

SET COLORIMETERS TO FULL SCALE, HIT RETURN
SET COLORIMETERS TO NORMAL OR PROPER DAMPING, HIT RETURN

All colorimeters being used must be adjusted, as directed, before hitting RETURN by using the adjustment knobs on the colorimeters.

The full-scale and baseline settings are recorded, allowing the computer input to be correlated with the recorder or digital printer (if used). It also tests the entire data-taking system and insures that it is working properly.

There are two possible error conditions. The first is due to inadequate range and give the following type of message applying to whichever colorimeter(s) needs attention:

DIFFERENCE BETWEEN F.S. AND NORMAL OF CHANNEL G, CL, READS LOW, .813621% F.S.
SHOULD READ 100% + OR - 10%, CHECK THAT INTERFACE IS ON, COLORIMETER CONNECTED AND TURNED ON

If nothing obvious is wrong, check with the computer coordinator. The program will again issue the prompts to set the colorimeter to full-scale. The second error condition gives a prompt as in this example:

NOT ENOUGH Ø OFFSET ON CHANNEL 7
READS 212 A/D COUNTS, SHOULD BE AT LEAST 400

This indicates the minor hardware problem that can easily be adjusted by the computer coordinator. It is important that there be sufficient zero offset so negative drift in baselines can be measured. The offset is usually set at 800 A/D counts.

Threshold Settings

The three set standards, especially the first, are critical to the automation procedure. The first set-standard peak establishes time delay to the peaks from sampling the first wheel location. A peak-threshold value is used to locate unequivocally the top of the set-standard peaks. This threshold value is used to signal that the peak is forming as it is increasing in height and that it is ending as it is decreasing in height. It is important that this value be chosen so that the first peak will always pass through the threshold value in both directions. In general, but not always, the set standards are chosen so that they produce a peak of one-half full-scale. A good threshold for this size peak is above 40% full-scale (TAASTART has been programmed for 39% for all analytes.) This is operator-variable, however, as can be seen by the next prompt:

THRESHOLD ON SET STND. OTHER THAN 39% ? *Y*

If answered *YES* then prompts ask for threshold values for each analyte, as for example:

THRESHOLD FOR SO4 ? *30*
THRESHOLD FOR CL ? *25.*

The *YES* response is necessary in many cases, for example, each analyte may require a different threshold value. When set standards produce higher or lower peaks, then higher or lower absolute thresholds will be needed. However, if chemistries are being run where there is very little separation between peaks, then relatively higher thresholds will have to be specified, that is, threshold values that are relatively closer to the expected height of the peaks. It is up to the operator to set threshold values that will insure detection of the first set-standard peak.

After appropriate threshold values have been specified, the following prompt appears: **HIT RETURN WHEN READY TO RUN.**

The pump is pumping, baseline looks good, and the three set standards are in position. When the RETURN key on the terminal is hit, **PEAK SEARCH BEGUN** is displayed. If any other message appears, there is a problem associated with the data entered in TAAIN, such as channel number, number of channels requested, number of samples per hour, or the number of data points per minute.

Error Messages

An error message with the following format could appear: **ERROR NUMBER Tn AT 410** where n is a number from 0 to 6. Table 2 shows a list of the different error codes and what they mean.

Example for error code T2:

The error code T2 might appear if the taking of data is so slow that all 35 data points are not recorded before the next peak comes along. As an example, the sampler is set at 40 samples per hour, which is 90 seconds per sample. If the data rate were set at 20 points per minute, then in 90 seconds only 30 points would have been taken, and the program expects to take 35 points per sample. The data rate can be increased as described on p. 12.

At this point the program is looking for the first set standard in order to establish the peak-to-sample-wheel location correlation. A 10-20-second pause will be noted, and then headers are displayed for up to three analytes such as:

SO4 **CL**

This pause is caused by program TAACAL being brought in from the disk. It does not interfere with the peak detection.

CALIBRATION

Set Standards

It is very important that the first set standard go above and then drop below 39% (or other specified value) of full-scale. Set standards should normally be chosen to give readings of 50% of full-scale so it is important to adjust the STD CAL knob on the colorimeter during the early part of the first peak to achieve this reading.

TABLE 2. List of error codes.

Code	Meaning
T∅	Floating point conversion error. Something has gone bad with the hardware. Call the computer coordinator immediately.
T1	Floating point conversion error. See T∅.
T2	Data-taking rate too slow for the number of samples per hour. See example following this list.
T3	Attempted to modify the timing on someone else's channel. This is highly unlikely. Inform your computer coordinator.
T4	Too many channels requested by all users. Presently the maximum is 18.
T5	Too many channels requested by one user. Presently the maximum is 6.
T6	The number of data points necessary to insure that a peak was located is too great. Someone has modified program TAASTART. Call your computer coordinator.

After the first set standard on all channels has been found, the following appears:

1 1 1 SET STND 1 47.39 47.38%

The first number is the record number in the file, the second is the wheel number (sample wheel), and the third is the position in the wheel (1 to 4∅). Next is the label, followed by a percent of full-scale for each peak. (For TAAO1, absorbance values appear.) This may not match your recorder exactly, but should be close. The peaks of the two remaining set standards are also read.

2 1 2 SET STND 2 48.13% 49.53%
3 1 3 SET STND 3 48.21% 49.48%
TIMING ERROR, SECS. ∅2.∅ -∅1.7

The timing-error message is not an error condition, but is printed at all times after the third set-standard peak has been read. This is the timing difference, in seconds, between the measured value from the second to third peaks and the calculated values from the response to the question **NUMBER OF SAMPLES PER HOUR ?**. If this number exceeds ±1∅ seconds you probably are in trouble. If it is likely that you might have entered the wrong value when asked **NUMBER OF SAMPLES PER HOUR ?** hit ESC and the question **DO YOU WANT TO STOP DATA TAKING ?** should be answered *Y*. You will then have to type *RUN"TAAIN*, and answer the questions that follow with a changed **NUMBER OF SAMPLES PER HOUR**. The computer-terminal dialogue to make the change is as follows:

RUN"TAAIN
DO YOU WANT TO RUN PREVIOUSLY STORED SAMPLE ID NOS. ? *N*
WHEEL PATTERN NO. (1 TO 9) *4*
IS THIS A RE-START OF AN INTERRUPTED RUN ? *Y*
DO YOU WANT TO ENTER NEW DATA
FOR EACH CHAN., QC PATT., STND. CONC., QC LIMITS

```
ANSWER ALL, SOME, OR NONE (A,S,N) ? S
WHICH VARIABLES DO YOU WANT TO CHANGE (Y OR N) ?

QCP          CS          SPK          STDS          DUP DIFF
? N          ? N         ? N          ? N           ? N

NUMBER OF SAMPLES PER HOUR ? 30
RUN NUMBER          5
    85          ID FILES IN LAST RUN
FIRST RECORD NO. 901
LAST RECORD NO. 985
SO4
CL
1       PATTERNS COMPLETED
2       PATTERNS COMPLETED
3       PATTERNS COMPLETED
4       PATTERNS COMPLETED
5       PATTERNS COMPLETED
85      FILES IN THIS SET UP
985     ID FILES IN USE
HEADER INFO ? N
EDIT FILES ? N
PRINT FILES ? Y
EDIT FILES ? N
ADDITIONS OR DELETIONS ? N
ANY OTHER CHANGES ? N
TAASTART 2809 05/24/77 13:20 800 DC
```

The sample-wheel pattern that prints out should be identical to the previous one. The run should then proceed normally.

Blanks

After the three set standards, two blanks are run to establish the baseline.

```
4    1    4    BLANK 1          0.13%          0.82%
5    1    5    BLANK 2          0.09%          0.71%
```

The computer will store the smaller of the two blanks to use for correcting subsequent readings.

Calibration Standards

The peak heights for the calibration standards are determined next. An example of the terminal output for the first calibration standard is shown below:

```
6    1    6    CAL STND 1       57.77%         71.56%
```

The displayed percentage of full-scale for each analyte has been corrected for baseline and should agree fairly closely with the recorder signal. Occasionally the warning

```
CAL STND NO. n ON y CHANNEL IS NOISY HIT ESC TO RESTART
```

is displayed, where n is the standard number and y is the name of the analyte. Look at the recorder trace of this peak. If it is obviously bad or the computer reading and the recorder reading differ significantly, you should stop the run, or there will be an error in all concentration calculations. Hit the ESC key, answer **DO YOU WANT TO STOP THE DATA TAKING ?** with a *Y*, reset the sample wheel to position number 1, fix the noise, and then type *RUN"TAASTART*. Make sure all peaks are out before restarting. If there is no signficant difference between the computed peak height and the recorded, leave it alone and after the run, check the standard deviation on the higher peaks as listed on the Final Operator Report to see if your allowable noise criterion is too stringent.

A second pair of blanks is run after the calibration standards, which is used to measure baseline drift, if any, during the run so far. A linear extrapolation is made between the lowest of these two blanks and the previous blanks and the extrapolated baseline subtracted from the calibration standards.

The concentration of the last blank of each set of blanks is calculated and compared to the previous set. If it exceeds the operator-selected difference, a buzzer sounds and the following message appears:

```
BASELINE DRIFT EXCEEDS ALLOWED ON SO4 CHANNEL
DRIFT = Ø.Ø73, ALLOWED = Ø.Ø5Ø
```

This message is given before the following message, which is always given for each set of blanks:

```
BLANK CONC., CL          NOW = Ø        PREV = Ø
BLANK CONC., SO4         NOW = -2       PREV = -2
```

> CAUTION!
> *DO NOT CHANGE THE ZERO CONTROL* on the colorimeter during an automated run. This will defeat the automatic correction features and give erroneous results.

After the second set of blanks has been run, the terminal displays the equations used to calculate concentration; for example,

```
CUBIC SOLUTION FOR SO4
C = -8.38E-Ø1 +3.Ø3E+Ø2*A/D-1.98E+Ø2*A/D↑2+1.97E+Ø2*A/D↑3
COEFF. OF DETN. + .998746
QUADRATIC SOLUTION FOR CL
C = +9.23E-Ø1 +1.Ø3E+Ø2*A/D+6.85E+Ø2*A/D↑2
COEFF. OF DETN. + .99953
```

The main program, TAA, is chained at this point. Its first function is to calculate the concentrations of the calibration standards as though they were samples.

		SO4		CL	
6	CAL STND 1	6	5	4	5
7	CAL STND 2	9	1Ø	9	1Ø
8	CAL STND 3	19	2Ø	19	2Ø
9	CAL STND 4	5Ø	5Ø	51	5Ø
1Ø	CAL STND 5	1ØØ	1ØØ	1ØØ	1ØØ

The first number under each analyte is the calculated concentration, and the second number is the known concentration. In conjunction with the coefficient of determination, these numbers give an indication of how well the curve fits the standards. In the case of interpolation, nothing is learned.

Calibration standards may be run in any order; the program then re-orders them since the calibration standards must be in ascending order of concentration for interpolation (as is done for SO4).

ANALYSIS

The main program (TAA) for sample analysis and concentration calculations has already been chained. The terminal-output format for all quality-control standards (check standards) is four lines of information.

Check Standards

The first "samples" in the QC pattern recognized by program TAA are the check standards.

```
12    1    12    CHK STND 1              46.83%              5Ø.69%
CONC. FOUND, MADE                    4.Ø5*      4      .514          .5
        DIFFERENCE                        .Ø5                  .Ø14
DIFF ALLOWABLE                            .2                   .Ø5
```

The *first* line is the peak height in percent full-scale. The *second* line for check standards shows the calculated concentration versus the known or made-up concentration. If the noise on the peak exceeds the criterion, an asterisk (*) appears after the calculated concentration. This indication is used for all solutions, samples, and standards alike. The *third* line is the difference between the measured and the made-up concentration and is expressed in absolute (unsigned) concentration units. The *fourth* line is the allowable difference as entered by the operator. If the measured difference exceeds the allowable, the following message will appear:

```
DIFFERENCE EXCEEDS ALLOWABLE FOR y, CHECK STANDARD n,
```

where y is the analyte name and n is the number of the check standard. A buzzer sounds also at this point.

Cumulative sums of the square of the difference (Cusums) and Shewhart limits are calculated and stored and appropriate messages stored for all quality-control standards. These data may be printed at the end of the run using TAAO4. A simple modification of the program can be made by the computer coordinator to allow these to be printed either in place of or in addition to the presently printed data.

Samples

The next QC-pattern data to be displayed at the terminal are the sample data. All sample data have the following format:

```
14    1    14    SMP 76Ø513              Ø2.35%              Ø1.62%
                 CONC.                      .21                 .Ø17
```

The sample identification is shown, along with the peak heights, on the *first* line. The *second* line is the concentration, which is rounded in two ways. Whereas in program TAAIN the prompt **PLACES AFTER DEC.** was answered with the maximum number of digits to appear to the right of the decimal, in TAA the numbers are

automatically rounded to three *digits* or less. For example, if the operator requests two places past the decimal:

Computed number	Displayed number
1.4784	1.48
Ø.Ø312461	Ø.Ø3
47.2163	47.2
871.563	872.

As with the check standard, an asterisk (*) next to the concentration will indicate a noisy peak. In the case of samples (and samples only) a message such as:

SAMPLE 76Ø429 AT POSITION 1 17 IS NOISY AND MUST BE RERUN PLACE IN POSITION 3 27

will appear. The suggested position would be the next available location in the last sample wheel.

If the sample is off-scale (1Ø% greater than the highest calibration standard), a double asterisk (**) will appear next to the concentration. Also, the following message will appear:

SAMPLE 76Ø327 AT POSITION 2 13 WAS DILUTED 1Ø NEED ADDITIONAL 4 TOTAL 4Ø PLACE IN POSITION 3 28

This message requests a REPEAT run of the sample.

The suggested dilution factor must be adhered to if you want the computer to calculate the concentration of the rerun correctly.

The above message does not appear for total Kjeldahl nitrogen (TKN), total phosphorus (TOTP) or chemical oxygen demand (COD). Since these samples usually require an external digestion step, an immediate dilution and rerun is impractical. (The ** does appear, however.)

If three asterisks (***) appear after the concentration, it means that the rerun of a sample was not successful. In addition, the following line will appear:

SAMPLE 76Ø317 AT POSITION 3 28 IS BAD FOR THE 2ND TIME

This means that the results are unacceptable either because the peak was noisy or off-scale. The sample will have to be rerun in another batch.

Spiked Samples

When the QC pattern contains spiked samples, the format for spiked samples is as follows:

24	1	24	SPK	76Ø513		23.65%			21.32%	
			CONC.			2.19			.216	
			RECOVERED	ADDED	1.98		2.Ø	.199		.2
			ALLOW. REC.,	MIN MAX	1.95		2.Ø5	.19		.21

The first two lines are similar to those of a sample. The identification of the sample to which the spike was added appears after SPK. Line three gives two pieces of information: the amount of the spike that was recovered (concentration of the spiked minus the concentration of the unspiked) and the amount of the spike added. If an asterisk (*) appears after the recovered amount, it means the unspiked sample was either noisy or off scale. The fourth line is a reminder of the allowable recovery as entered by the operator.

If the amount recovered does not meet the criterion, the following line appears:

RECOVERY LESS THAN ALLOWABLE FOR SULFATE, SPIKE 76Ø321

or a similar message with **MORE** replacing **LESS**. The message is accompanied by a buzzer.

Duplicates

Output at the terminal for duplicate data has the following format:

36	**1**	**36**	**DUP**	**76Ø427**	**Ø8.17%**	**Ø9.34%**
			CONC.		**.81**	**.Ø93**
DIFF. DIVIDED BY DIL					**.Ø2**	**.ØØ4**
			DIFF. ALLOWABLE		**.Ø5**	**.Ø1**

The format of the first two lines is identical to that of a spike. The third line is the absolute (unsigned) difference in concentration units between the duplicates divided by the dilution factor. An asterisk (*) after the difference indicates a problem was encountered with the data for the first sample of the pair. The fourth line indicates the allowable difference in duplicates (DIFF IN DUPS) as entered by the operator.

Completion of a duplicate analysis marks the end of the analyses for a given QC pattern. Analysis then continues for all the remaining QC patterns until all solutions in the run have been completed. Terminal results and messages are repeated for each QC pattern in the sequence just described above in the section on analysis.

Messages

Timing Change. Often, during the analyses of samples with TAA, the following type of message appears:

TIMING CHANGE ON SO4 CHAN. OR 5.99998 SEC.

This message informs the operator that the peak-to-peak timing has automatically been corrected for timing errors that have accumulated during the preceding analysis periods. It was mentioned previously that peak-to-peak timing is based on a constant value, not peak detecton. The constant is adjusted however, by a peak detection algorithm that examines the distribution of data points about the peak. (See Volume 2 of this document, Notes to Coordinator.) If the algorithm calculates that the peak is arriving too soon or too late, a timing change is calculated.

BASIC Messages. Occasionally, BASIC will detect an error of some kind and will print a message such as:

ERROR NO. 16 AT LINE 764Ø—ARITHMETIC

The program stops as a result of attempting to divide by ∅. The operator should type on the console *LIST nnnn* where nnnn is the line number in the error statement. You might try to continue by typing *CON*. Make a note of the error number, line number, and the response when *LIST nnnn* is typed. It could be a software problem; call your computer coordinator. Various other diagnostic messages may appear from time to time, which are discussed in Volume 2.

When all samples and repeats are complete, the program will automatically start the sequence of programs to prepare the preliminary and notebook reports.

Interrupting a Run

While running samples with TAA, it may be necessary to interrupt the run before all solutions have been analyzed. Interrupting may be required (1) if the operator wishes to obtain a list of all samples that need repeat runs due to noisy or off-scale signals, (2) the instrument requires minor repair, or (3) reagents need to be replaced. The run can be stopped by hitting ESC (once only!). The following message with options appears at the terminal:

PLEASE SELECT ONE OF THE FOLLOWING OPTIONS BY TYPING BRACKETED LETTERS
LIST REPEATS [RPT], RESTART WITH STANDARDS [STY],
RESTART WITHOUT STANDARDS [STN],
STOP DATA TAKING, GET REPORT [SWR], STOP DATA TAKING, NO REPORT [SNR],
OR CONTINUE DATA TAKING, STOP BASIC PROGRAM [SBP]

The operator then types the desired 3-letter option after the ? prompt. These are explained below:

List Repeats

? *RPT*

Although the computer sounds a buzzer and prints a warning every time an off-scale or noisy peak is encountered, the operator may not be available at the time. In the case of cathode ray tube (CRT) terminals, these warnings may well have scrolled off the top of the screen before the operator sees them. To get a list of all the samples that need rerunning, type *RPT*. Possible responses are shown.

CONGRATULATIONS! NO REPEATS.

or

NOT BAD, ONLY 2 REPEATS

48	**2**	**8**	**SMP**	**1∅1**	**NOISY**
49	**2**	**9**	**SMP**	**1∅2**	**DIL. ADDITIONAL 4 TOTAL DIL. 4∅**

or

TOO BAD, THERE ARE 14 REPEATS

48	**2**	**8**	**SMP**	**1∅1**	**NOISY**
49	**2**	**9**	**SMP**	**1∅2**	**NOISY**
5∅	**2**	**1∅**	**SMP**	**1∅3**	**NOISY**
51	**2**	**11**	**SMP**	**1∅4**	**NOISY**
52	**2**	**12**	**SMP**	**1∅8**	**NOISY**
53	**2**	**13**	**SMP**	**1∅9**	**NOISY**
54	**2**	**14**	**SMP**	**11∅**	**NOISY**
55	**2**	**15**	**SMP**	**111**	**NOISY**
56	**2**	**16**	**SMP**	**112**	**NOISY**

```
57    2    17    SMP    113    NOISY
58    2    18    SMP    114    NOISY
59    2    19    SMP    115    NOISY
6Ø    2    2Ø    SMP    119    NOISY
61    2    21    SMP    12Ø    NOISY
```

The number of repeats is shown followed by the record number, the wheel number, the position in the wheel, the sample identification and either a suggested dilution or **NOISY**.

Restart with Standardization

```
? STY
LAST GOOD RECORD NO. ? 949
GET OUTPUT FROM LINEPRINTER, THEN RUN TAAIN.
USE RE-START OPTION IN TAAIN
```

In this example the operator noticed that erratic data started being generated part-way through the run. Examination of terminal output showed that data for record number 949 was the last good analysis. It was decided to restart at record 95Ø with standardization. To do this, the operator must relocate the calibrate-pattern solutions in the sample-wheel pattern so that they occupy the wheel locations just ahead of the solution specified by record number 95Ø. The wheel must then be located with the first set standard at the sampling position.

TAAIN must now be run to inform the computer of the new configuration of the sample wheel pattern:

```
*RUN"TAAIN
DO YOU WANT TO RUN PREVIOUSLY STORED SAMPLE ID NOS. ? N
WHEEL PATTERN NO. (1 TO 9) 4
IS THIS A RESTART OF AN INTERRUPTED RUN ? Y
DO YOU WANT TO ENTER NEW DATA
FOR EACH CHAN., QC PATT., STND. CONC., QC LIMITS
ANSWER ALL, SOME, OR NONE (A,S,N) ? N
RUN NUMBER          8
    49 ID FILES IN LAST RUN
FIRST RECORD NO. 95Ø
LAST RECORD NO. 985
SO4
CL
1 PATTERNS COMPLETED
2 PATTERNS COMPLETED
4Ø FILES IN THIS SET UP
989 ID FILES IN USE
HEADER INFO ? N
EDIT FILES ? N
PRINT FILES ? Y
EDIT FILES ? N
ADDITIONS OR DELETIONS ? N
```

ANY OTHER CHANGES ? *N*
TAASTART 2809 05/24/77 13:20 800 DC

The prompts must be answered as shown with the restart option answered *YES*, and the record number of the first sample to be run and the last record number of the *original* wheel pattern; do not include repeat samples.

The first question regarding previously stored IDs must be answered *NO* even though previously stored IDs are being used!

Restart without Standardization

? *STN*
DO NOT RESTART ON BLANKS, SPIKES OR DUPLICATES
RECORD NO. OF FIRST RUN ON RESTART ? *950*
NO. OR REAGENT BLANKS RUN BEFORE THIS RECORD ? *0*
WANT TO RUN ALL, SOME OR NONE OF REPEATS ALREADY ASKED FOR [A,S,N] *S*
HOW MANY TO BE USED (IN ORDER FROM 1ST) ? *3*
PLACE A SET STANDARD IN THE POSITION
JUST BEFORE THE FIRST SAMPLE TO BE RUN
LOCATE THE SAMPLE WHEEL TO SAMPLE THE SET STANDARD
THRESHOLD ON SET STND. OTHER THAN 39% ? *Y*
THRESHOLD FOR SO4 ? *35*
THRESHOLD FOR CL ? *30*
HIT RETURN WHEN READY TO RUN

It is not necessary to use TAAIN when restarting without standardization. All that is required is to answer the prompts shown above. The prompts regarding REPEATS allow the operator to select only those repeats that occurred during the "good" portion of the run. It should be noted that a set standard is placed just before the first sample to be run, and the sample wheel located to sample the set standard. After hitting RETURN, the next message will be **PEAK SEARCH BEGUN**, and **DATA** about the set standard will not appear.

Stop Data Taking, with Report

? *SWR*
LAST GOOD RECORD NO. ? *949*
TOTAL NO. OF REPEATS RUN ? *0*
TAA01 5283 05/25/77 10:37 3090 DC
SETTING UP FILES FOR SUMMARY DATA REPORT

This option allows the operator to stop data-taking and obtain a report for all the good analytical results up to and including the specified record number. Also, in the unlikely event that the run has been stopped after some repeat runs have been made, the report will include the results for good repeats. Use of this option implies no further analyses of the remaining samples will be made at this time. They will be included in a later work session.

Stop Data Taking, No Report

? SNR
STOP AT 2988
*

When all data appear to be bad because all samples need dilution or there is a system or instrument malfunction, this option stops everything. No report is made. Appropriate corrective action must be taken before restarting. If you later decide you would like to print the data, use program TAAPRINT.

Stop BASIC Program, Continue Taking Data

? SBP
TYPE CON TO RETURN

This option should be used only by an extremely skilled and experienced operator. It allows the operator to make a minor modification of the BASIC program, SAVE it, read out some variables, list on the line printer, etc. These operations must all be done in three sample periods (the time between four peaks) or data will be missed. When the modification has been made, typing *CON* will bring up BASIC and the program will continue as if nothing has happened, if the operator was fast enough.

POSTANALYSIS PROCEDURES AND LINE PRINTER REPORTS

SCOPE

After data peaks for all solutions in the sample-wheel pattern have been read by the TAA program, four programs are used to provide the necessary printed output of the collected data. The programs, which are chained together, are TAAO1, TAAO2, TAAO3, and TAAO4. They perform four tasks: print preliminary analysis results, allow reagent-blank corrections, print summary data report, and print a Cusum and Shewhart QC data report.

PROGRAM TASKS

Preliminary Analysis Results (TAAO1)

If reagent blanks have been used, TAAO1 compiles and prints out a report of "Preliminary Analysis Results" and chains to TAAO2. If reagent blanks have not been used it sets up data files and chains to TAAO3.

The preliminary report comprises data for all the individual solutions that make up a work session including the sequence of set standards, blanks, calibration standards, samples, check standards, reagent blanks, spikes, duplicates, and samples that have been rerun. It lists in sequence each solution, the identification of the solution and the peak height and concentration. The operator uses the report to compare that data with data for reagent blanks that will subsequently be displayed on the terminal. It aids him/her in judging the quality of reagent-blank data so that he/she can decide how to use the reagent blanks.

Reagent-Blank Corrections (TAAO2)

Corrections for reagent blanks are made interactively by the operator. TAAO2 retrieves, in sequence, data for each reagent blank and displays the data on the terminal. The run number, the reagent-blank number, the peak height and the concentration for each analyte of the run, and the samples to which the

blank applies are shown. The program issues prompts asking whether the data are all right, and if the operator wants to subtract the reagent-blank value from the samples to which it applies. The operator will make a judgment and respond to the prompts after comparing the reagent-blank data with that contained in the preliminary report for instrument blanks, samples, etc. After the operator responds, the program will then proceed to the next reagent blank and the process will be repeated until all of the reagent blanks have been retrieved, displayed, and acted upon. Finally the TAAO2 program will display a summary review of the actions taken on all of the reagent blanks retrieved for the work session.

Summary Data Report (TAAO3)

TAAO3 compiles and prints out a "Summary Data Report." The report lists the runs in sequential order, and for each run prints the data across the page including the run number, the identification of the run, the peak height and standard deviation of the peak, the dilution factor (where applicable) and the concentration. These data can be printed for a maximum of three analytes across the page. In addition, the report gives a one-digit code number indicating the quality of the result for each run and for each analyte (See Table 3). These code numbers are printed in the right-most column under "COMMENT." A table is provided on each Summary Data Report to enable interpretation of the quality code numbers.

The report also contains information about standards, samples, and quality controls. It also prints out standard-calibration coefficients, and degree, goodness of fit, and quality-control values for check standards, spikes, and duplicate samples. TAAO3 then chains to TAAO4, if desired.

Cusum and Shewhart QC Data Report (TAAO4)

TAAO4 compiles and prints out the Cusum and Shewhart QC Data Report. The report lists the QC data for check standards, spikes and duplicates. All of the data for the first channel are listed first followed by each succeeding channel. The Cusum and Shewhart warning messages, where applicable, are also listed.

This program is not used by all laboratories.

TABLE 3. List of comment codes.

0	Good data
1	Out of calibrate, offscale
2	Noisy peak
3	Good analyte in repeat
4	Bad 2nd time
5	Bad QC, otherwise good
6	Bad standard, bad QC
7	Spiked or duped bad, bad QC
8	Spiked or duped bad, QC OK
9	Not analyzed (peak missed)

RUNS WITHOUT REAGENT BLANKS

If reagent blanks have not been used the TAAO1 program is chained in at the end of the work session by the TAA program. After TAAO1 sets up data files, TAAO3 and TAAO4 are chained in sequentially. As these programs are chained in, the following messages appear:

```
SETTING UP FILES FOR SUMMARY DATA REPORT                (TAAO1)
SUMMARY DATA REPORT PROGRAM IS RUNNING                  (TAAO3)
SUMMARY DATA REPORT IS COMPLETED
GET REPORT FROM THE LINE PRINTER
CUSUM AND SHEWHART REPORT PROGRAM RUNNING               (TAAO4)
CUSUM AND SHEWHART DATA REPORT IS COMPLETED
GET REPORT FROM LINEPRINTER
END AT 1580
```

No further interaction is required by the operator. The work session is complete. The data remain available until a new run is initiated using the same wheel number. To produce another copy of the data, use TAAPRINT.

RUNS WITH REAGENT BLANKS

If reagent blanks have been used, the first message appearing at the terminal is:

```
GET PRELIMINARY REPORT FROM THE LINEPRINTER.
```

At this point TAAO2 is chained in as indicated by the following messages:

```
THE FOLLOWING ARE REAGENT BLANKS IN THIS SERIES OF RUNS
DETERMINE THEIR USE
COMPARE THE FOLLOWING DATA WITH PRINTOUT OF PRELIM ANALYSIS
```

The program goes out to the files and looks for reagent blanks in each pattern of samples, check standards, spikes, and duplicates. It also looks for reagent blanks in the first grouping of set standards and calibration standards (even though reagent blanks are not normally included in the first grouping). Thus, the program will virtually always display the following message first:

```
NO REAGENT BLANKS FOUND IN GROUP 1
```

When a reagent blank is found in a pattern the following information, for example, is displayed:

```
RUN   15   RB   2
PH          CON          PH          CON
.14%        0.0034       .02%        0.0005
THIS REAGENT BLANK APPLIES TO SAMPLES 1 TO 3 AND SAMPLES 4 TO 6.
```

(The symbols PH and CON refer to peak height and concentration.) The program will then ask:

IS THE REAGENT BLANK OK ? *Y*

The operator will make a judgment (by comparing the displayed values with pertinent data in the preliminary report) and respond *Y* or *N*. The program will then ask:

WANT TO ENTER MANUAL RB CONC. ?

With this prompt the operator can elect to enter a reagent-blank concentration he/she has estimated or calculated manually. If the operator responds with *Y*es, the computer will prompt him/her with a question mark under each computer-calculated RB concentration and the operator should enter the estimated concentration. If *N*o is the answer, the next prompt is:

DO YOU WANT TO SUBTRACT THE REAGENT BLANK ? *N*

The operator will again make a judgment and respond *Y* or *N*. The program will retrieve any additional reagent blanks in the pattern; the query, judgment, and response process is repeated. When all reagent blanks in the pattern are retrieved, the following message is then displayed:

REAGENT BLANKS RETRIEVED FROM GROUP 2

The program will then retrieve reagent blanks in the next pattern, and the process is again repeated until all reagent blanks in all of the patterns are retrieved and acted upon. The following message is then displayed:

ALL REAGENT BLANKS RETRIEVED.

Finally a summary review of all the actions taken on all of the reagent blanks in the entire series of runs that make up the work session will be displayed as follows:

SUMMARY REVIEW OF ALL REAGENT BLANKS IN THIS SERIES OF RUNS COMING UP
RUN 15 RB 2
PH CON PH CON
.14% Ø.ØØ34 .Ø2% Ø.ØØØ5
RB OK, NOT SUBTRACTED
REVIEW OF REAGENT BLANKS COMPLETE

TAAO3 is then chained in by the TAAO2 program. At the outset the TAAO3 program displays the message:

SUMMARY DATA REPORT PROGRAM IS RUNNING

and is followed by the same messages described in the section on Runs without Reagent Blanks, above.

The program retrieves, from a variety of files, all of the information necessary to print the Summary Data Report. The information is sent out to the line printer in patterns (preceded by the grouping of set standards and calibration standards) as previously described. Each pattern is printed on a new page.

SPECIAL PROGRAMS

There are three diagnostic or recovery programs written for use with the TAA programs. It may be useful for the operator to understand how to use them.

TAAPRINT

This is a simple, short program that sets up variables necessary for printing final results. This program is only needed when the system crashes to save useful data that have already been created. A typical dialogue follows:

RUN"TAAPRINT
FIRST RECORD NO. *1*
LAST GOOD RECORD NO. *48.*
NO. OF RBL'S RUN *0*

At this point TAAO1 is chained in and the normal printing sequence begins.

TAAPEAK

This program is an extremely useful diagnostic tool for examining the raw data used in calculating peak heights. Typically, 35 readings from the A/D are taken for each peak from the TAA. These raw data are stored in a sequential file, PTSX, where X is 1, 2, or 3, depending on how many channels are being run together, and the number of the analyte (sequential number as entered by the operator). As an example, if two channels were used and the operator entered CL first and SO4 second, PTS1 would be the chloride data and PTS2 the sulfate.

This program displays the raw data semigraphically on the line printer. It can help spot noise, shifts in timing, or help to set data rates. The dialogue for running this program is as follows:

RUN"TAAPEAK
ANALYTE NUMBER (1 to 3) *1*
FIRST PEAK NO. *5*
LAST PEAK NO. *13*

At this point the data are read from the file into a large array, the highest and lowest points are found (for scaling), and the peaks requested are printed. If the PAGE has not been set to 132, either arrows will occur or the data will be very strange.

TAAPFILE

This program is used to print the contents of file TAAID.XX (where XX is the first two letters of the analyte) in a formatted, easy-to-read way. The contents of this file are adequately described in Vol. 3 of this document "File Structure for Technicon AutoAnalyzer."

The dialogue to run is as follows:

RUN"TAAPFILE
1ST RECORD, LAST *5,27*

Again it is important that PAGE be set at 132 for this program to run. It will automatically print the files for all analytes.

JK

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